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Industry-Wide Workshop on Computational Turbulence Modeling

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sponsored by the
Institute for Computational Mechanics in Propulsion
and Center for Modeling of Turbulence and Transition
Ohio Aerospace Institute
Cleveland, Ohio
October 6-7, 1994*



National Aeronautics and
Space Administration

Office of Management

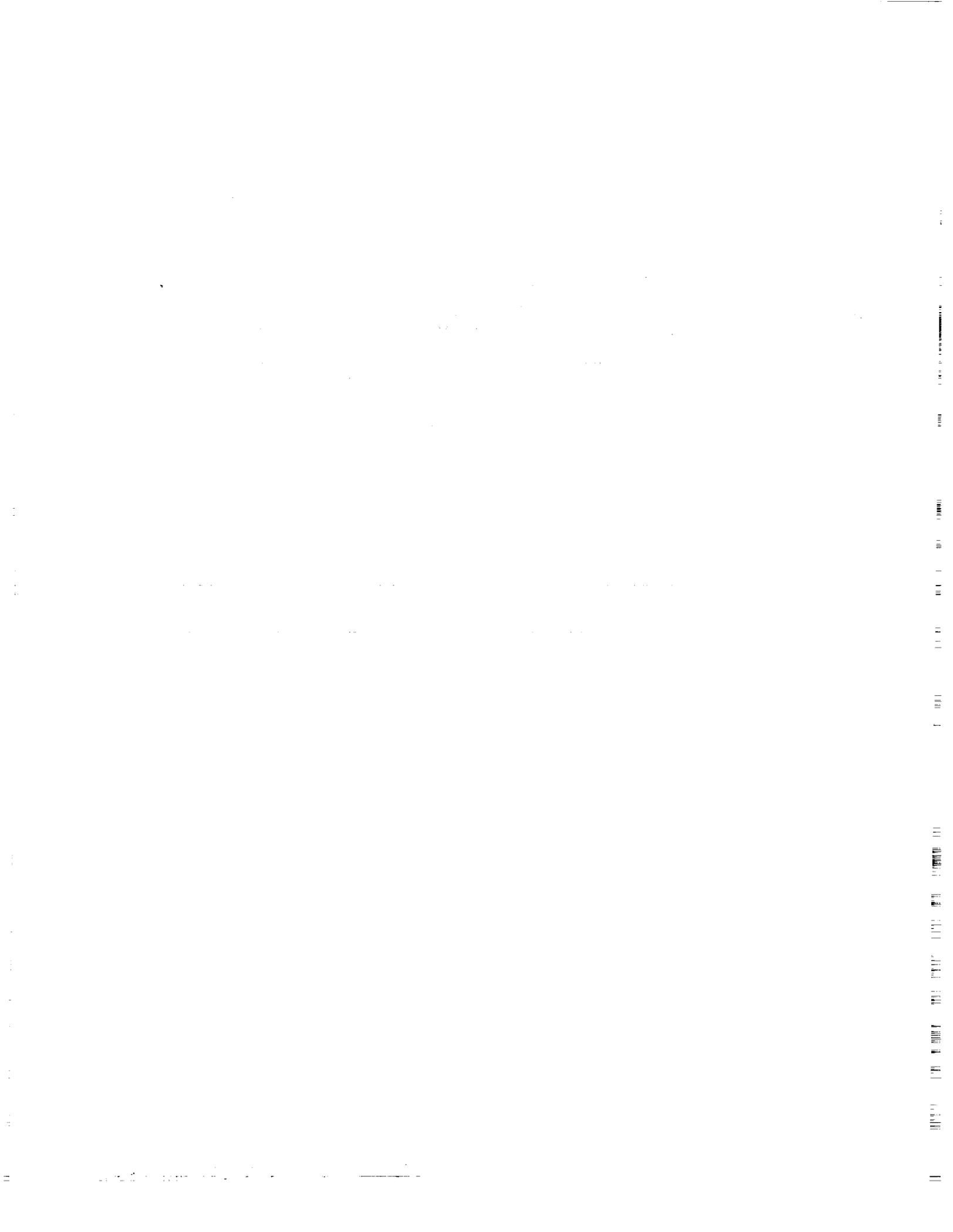
Scientific and Technical
Information Program

1995

Preface

This publication contains the presentations made at the Industry-wide Workshop on Computational Turbulence Modeling, which was hosted by ICOMP/LeRC, and took place on October 6-7, 1994 at the Ohio Aerospace Institute. The purpose of the workshop was to initiate the transfer of technology developed at Lewis Research Center (LeRC) to industry and to discuss the current status and the future needs of turbulence models in industrial CFD. To address the latter, a total of fourteen presentations were made by researchers from industry. CMOTT would like to thank all the workshop speakers for bringing to our attention a host of problems which are important to industry and for which they think CMOTT can be of help. We are prioritizing all the suggestions in order to incorporate them into the CMOTT work plan.

One unanimous recommendation of the workshop participants was to make the workshop an annual event. This first workshop grew out of the recommendations by the peer review committee of the LeRC turbulence modeling program, held in September of 1993. It could have not successfully transpired without the help and guidance of Dr. Chander Prakash (GE-Aircraft Engines), Dr. Munir Sindir (RocketDyne), and Dr. Saadat Syed (Pratt & Whitney), and for this CMOTT would like to thank them.



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TABLE OF CONTENTS

TURBULENCE PROGRAM FOR PROPULSION SYSTEMS Tsan-Hsing Shih, Institute for Computational Mechanics in Propulsion and Center for Modeling of Turbulence and Transition, NASA Lewis Research Center	1
TURBULENCE MODEL DEVELOPMENT AND APPLICATION AT LOCKHEED FORT WORTH COMPANY Brian R. Smith, CFD Group, Lockheed Fort Worth Company	29
A SUMMARY OF COMPUTATIONAL EXPERIENCE AT GE AIRCRAFT ENGINES FOR COMPLEX TURBULENT FLOWS IN GAS TURBINES R. Zerkle and C. Prakash, GE Aircraft Engines	39
THE APPLICABILITY OF TURBULENCE MODELS TO AERODYNAMIC AND PROPULSION FLOWFIELDS AT McDONNELL DOUGLAS AEROSPACE Linda D. Kral, John A. Ladd, and Mori Mani, McDonnell Douglas Aerospace	47
EXPERIENCE WITH $k-\epsilon$ TURBULENCE MODELS FOR HEAT TRANSFER COMPUTATIONS IN ROTATING Prabhat Tekriwal, GE Corporate Research and Development	65
TURBULENCE MODELS FOR GAS TURBINE COMBUSTORS Andreja Brankovic, CFD Group, Pratt & Whitney	79
COMBUSTION SYSTEM CFD MODELING AT GE AIRCRAFT ENGINES D. Burrus and H. Mongia, GE Aircraft Engines, and A. Tolpadi, S. Correa, and M. Braaten, GE Corporate Research and Development	87
RECENT PROGRESS IN THE JOINT VELOCITY-SCALAR PDF METHOD M.S. Anand, Allison Engine Company	99
OVERVIEW OF TURBULENCE MODEL DEVELOPMENT AND APPLICATIONS AT ROCKETDYNE A.H. Hadid, E.D. Lynch, and M.M. Sindir, Rocketdyne Division, Rockwell International	107
RECENT ADVANCES IN PDF MODELING OF TURBULENT REACTING FLOWS A.D. Leonard and F. Dai, CFD Research Corporation	119
EXPERIENCE WITH TURBULENCE INTERACTION AND TURBULENCE-CHEMISTRY MODELS AT FLUENT INC. D. Choudhury, S.E. Kim, D.P. Tselepidakis, and M. Missaghi, Fluent Inc.	131
EXPERIENCES WITH TWO-EQUATION TURBULENCE MODELS Ashok K. Singhal, Yong G. Lai, and Ram K. Avva, CFD Research Corporation	143
PROGRESS IN SIMULATING INDUSTRIAL FLOWS USING TWO-EQUATION MODELS: CAN MORE BE ACHIEVED WITH FURTHER RESEARCH? Vahé Haroutunian, Fluid Dynamics International, Inc.	155

TURBULENCE MODELING NEEDS OF COMMERCIAL CFD CODES: COMPLEX FLOWS IN THE AEROSPACE AND AUTOMOTIVE INDUSTRIES	
Bizhan A. Befrui, adapco	171
TURBULENCE REQUIREMENTS OF A COMMERCIAL CFD CODE	
J.P. Van Doormaal, C.M. Mueller, and M.J. Raw, Advanced Scientific Computing Ltd.	193
SECOND-ORDER CLOSURES FOR COMPRESSIBLE TURBULENCE	
J.L. Lumley, S. Savarese, and C.C. Volte, Mechanical and Aerospace Engineering Department, Cornell University	203
MODELING OF TURBULENT CHEMICAL REACTION	
J.-Y. Chen, Department of Mechanical Engineering, University of California, Berkeley	219
INTRODUCTION TO TURBULENCE SUBPROGRAM	
T.-H. Shih and J. Zhu, Institute for Computational Mechanics in Propulsion and Center for Modeling of Turbulence and Transition, Lewis Research Center	231
DESCRIPTION OF TURBULENCE SUB-PROGRAM	
J. Zhu, Institute for Computational Mechanics in Propulsion, NASA Lewis Research Center	235
OVERVIEW OF PROBABILITY DENSITY FUNCTION (PDF) MODELING AT LeRC	
D.R. Reddy, Internal Fluid Mechanics Division, NASA Lewis Research Center	243
PDF METHODS FOR TURBULENT REACTIVE FLOWS	
Andrew T. Hsu, NYMA, Inc., NASA Lewis Research Center	247
A COMPOSITION JOINT PDF METHOD FOR THE MODELING OF SPRAY FLAMES	
M.S. Raju, Nyma, Inc., NASA Lewis Research Center	259
IMPROVEMENTS AND NEW FEATURES IN THE PDF MODULE	
A.T. Norris, Institute for Computational Mechanics in Propulsion	269
ATTENDEES LIST	277

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BACKGROUND

- CMOTT group at LeRC has been in existence for about 4 years. In the first 3 years, its main activities were in developing and validating turbulence and combustion models for propulsion systems, in an effort to remove the deficiencies of the existing models. Two workshops on computational turbulence modeling were held at LeRC (1991, 1993).
- A peer review of turbulence modeling activities at LeRC was held in September, 1993. Seven peers (GE, P&W, RocketDyne, Cornell, Berkeley and NASA Ames) conducted the peer review. The objective of the peer review was to assess the turbulence program at LeRC/CMOTT and to suggest the future direction of turbulence modeling activities for propulsion systems.
- Important messages from the peer review:
 - ◇ “LeRC should spend substantial effort being responsive to industry’s current pressing perceived needs; this involves extensive discussion with industry during every phase of model development, analysis of industry’s problems, goal oriented model development, evaluation of models relative to industry’s intended application ...”
 - ◇ “LeRC has an obligation not only to respond to industry’s requests for help, but to play an autonomous, independent leadership role in providing models of the highest quality, ... which can be employed not only by the aircraft gas turbine and rocket industries but also by other industries ...”
 - ◇ “In the present financial climate, industry does not have the resources to undertake model development and evaluation. LeRC’s help in this regard via the creation of its turbulence modeling effort, is, therefore, welcome from the industry’s standpoint.”
 - ◇ “It is important to work with the industry to evaluate the models and rank-order them by performance and cost in order to identify the most appropriate models for particular situations.”
 - ◇ Many other useful suggestions and comments including collaboration with industry, joint programs, industry-wide workshop ...

PROGRAM GOALS AT CMOTT

- Develop reliable turbulence (including bypass transition) and combustion models for complex flows in propulsion systems
- Integrate developed models into deliverable CFD tools for propulsion systems in collaboration with industry.

PROGRAM APPROACH

- Develop turbulence and combustion modules for industry customers
- Industry collaboration and technology transfer
- Model development for propulsion systems
 - ◇ One-point moment closures for non-reacting flows
 - ◇ Scalar PDF method for turbulent reacting flows
 - ◇ Validation of existing and newly developed models

Development of Turbulence and Combustion Modules

- Objective
 - ◇ Build a quick and efficient vehicle for technology transfer to industry
- The features of the turbulence module:
 - ◇ It contains various turbulence models from which users can choose the appropriate model for flows of interest
 - ◇ It is self-contained, i.e., it contains its own solver for turbulence model equations
 - ◇ It can be easily linked to industry's CFD codes
- Turbulence module for NPARC code has been developed, tested, and is ready to be released
 - ◇ The models built-in at the present time:
Mixing length, Chien $k - \epsilon$, CMOTT $k - \epsilon$ models
 - ◇ The model to be built-in:
CMOTT algebraic Reynolds stress, Reynolds stress transport equation models and other models based on the request from industries.
 - ◇ Built-in robust, realizable numerical solver for model equations.
- General turbulence modules
 - ◇ Can be used for both compressible and incompressible flows.
 - ◇ Interface programs for different industry CFD codes
 - ◇ Built-in models will be periodically updated.

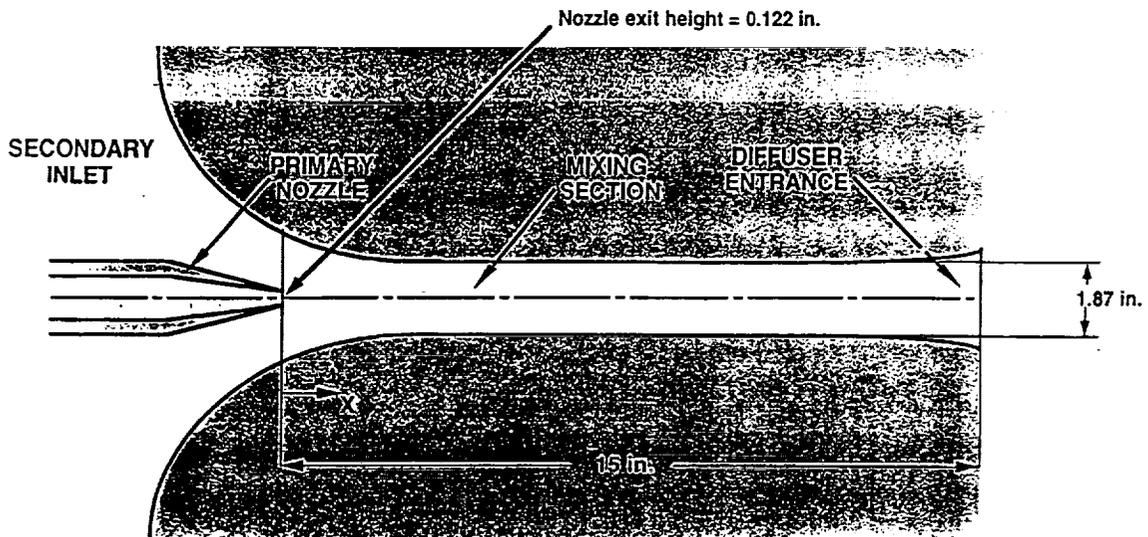
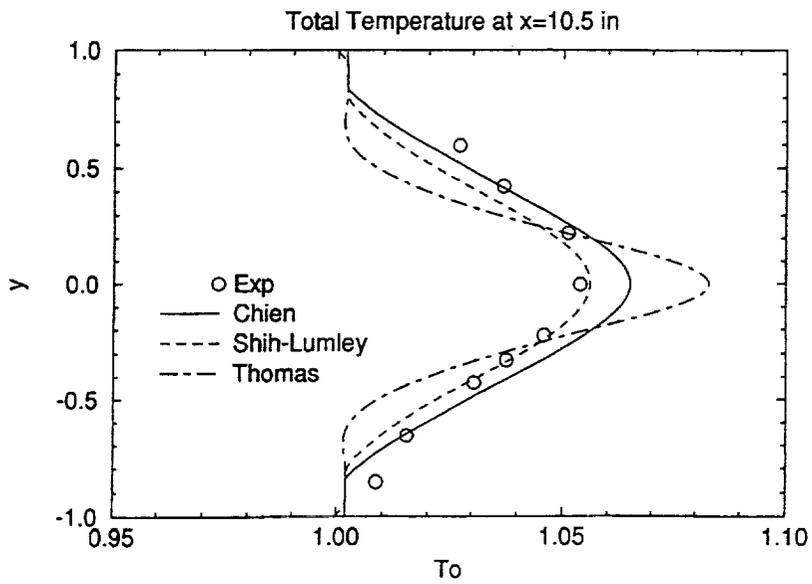
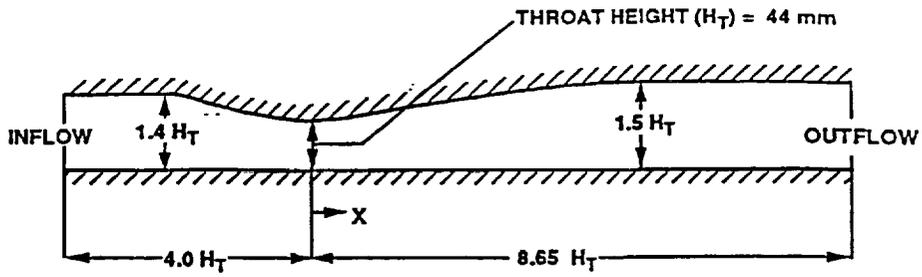
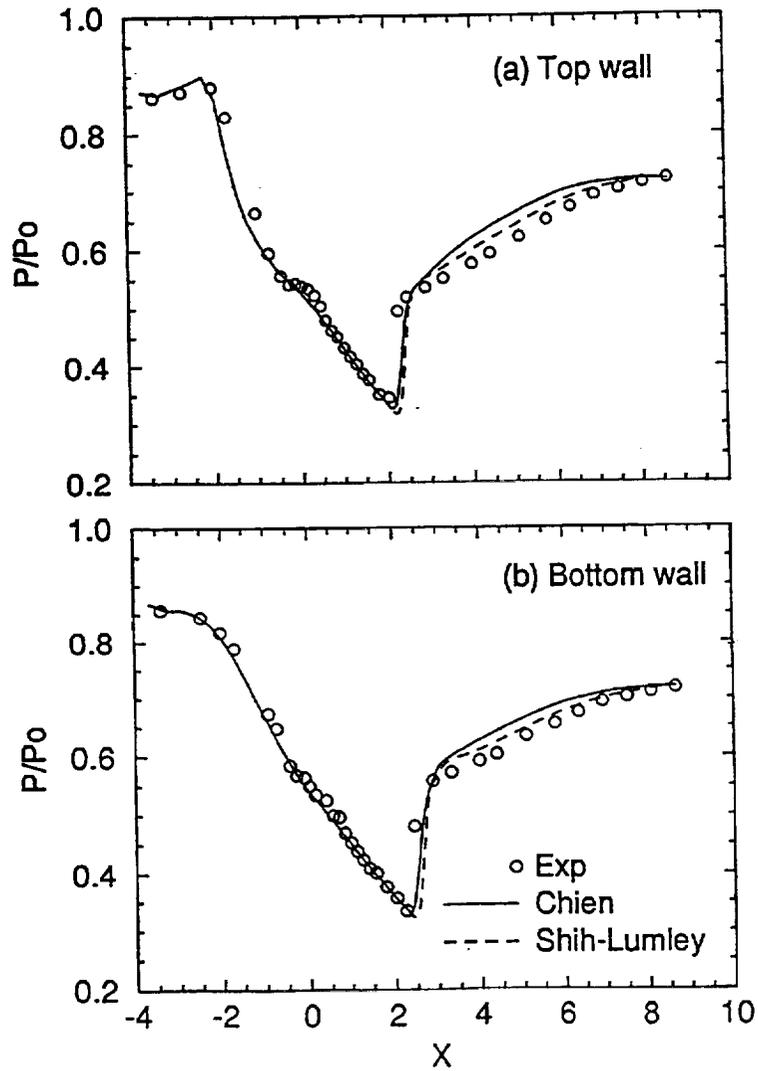


Fig. 3. Schematic of ejector nozzle test case.





Strong-shock case



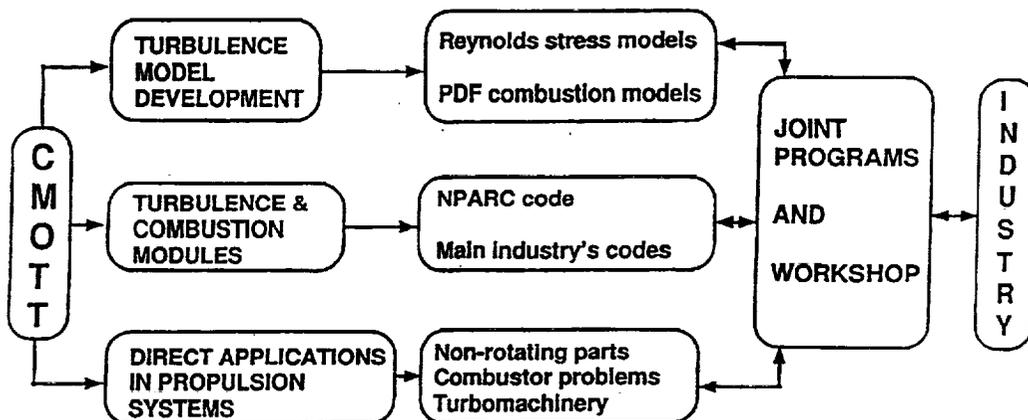
Collaboration with Industry and Technology Transfer

- Joint research programs with industry
 - ◇ Preliminary programs with engine companies and others have been initiated (GE, P&W, RocketDyne, Naval Research Laboratories)
 - ◇ Develop further joint research programs related to the industry's projects
- Industry-wide workshops will be a regular program (once every two years)
 - ◇ Release Lewis turbulence and combustion modules to industries
 - ◇ Discuss the needs of industry

Models developed at CMOTT

1. Isotropic eddy viscosity models
2. Reynolds stress & scalar flux algebraic equation models
3. Second moment transport equation models
4. Multiple-scale models for compressible turbulent flows
5. Bypass transition models
6. PDF models for turbulent reacting flows

PROGRAM SUMMARY



Isotropic eddy viscosity models

- Objective

- ◇ To examine the deficiencies of existing models
- ◇ To develop better eddy viscosity models

- Current status of existing $k - \epsilon$ eddy viscosity models

$$-\overline{u_i u_j} = \nu_T (U_{i,j} + U_{j,i}) - \frac{2}{3} k \delta_{ij}, \quad \nu_T = C_\mu f_\mu \frac{k^2}{\epsilon}$$

$$\frac{Dk}{Dt} = T^{(k)} + P^{(k)} - \epsilon + \text{W.C.}, \quad \frac{D\epsilon}{Dt} = T^{(\epsilon)} + P^{(\epsilon)} - D^{(\epsilon)} + \text{W.C.}$$

- ◇ They are not tensorially invariant due to $f_\mu(y^+)$, $\text{W.C.}(y^+)$
 - ◇ Model constants are not consistent for flows with and without wall
 - ◇ Normal stresses may violate realizability
 - ◇ Do not work very well for flows with pressure gradients
- Development of a Galilean-, tensorially invariant, realizable, $k - \epsilon$ model
 - ◇ New damping function $f_\mu(k/S\nu)$ is proposed to remove the dependence on y
 - ◇ New dissipation ϵ equation is introduced to give better response to pressure gradients
 - ◇ Consistent model coefficients for all flows
 - ◇ Realizability of the normal stresses is guaranteed
 - ◇ Modified wall function for cases with pressure gradients

- CMOTT $k - \varepsilon$ eddy viscosity model

$$-\overline{u_i u_j} = \nu_T (U_{i,j} - U_{j,i}) - \frac{2}{3} k \delta_{ij}, \quad \nu_T = C_\mu f_\mu \frac{k^2}{\varepsilon}$$

$$\frac{Dk}{Dt} = T_k + P_k - \varepsilon$$

$$\frac{D\varepsilon}{Dt} = T_\varepsilon + C_1 f_1 S \varepsilon - C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} + f_\phi \Phi$$

- ◇ f_μ, f_1, f_ϕ are functions of $R = k/S\nu$, which is tensorially invariant
- ◇ $C_\mu = \frac{1}{A_0 + A_* U_* k/\varepsilon}$, which ensures realizability for normal stresses
- ◇ Φ represents the effect of inhomogeneity

$$\Phi = b_1 \nabla k \nabla k + b_2 \frac{k^2}{\varepsilon} \nabla S \nabla k + b_3 \frac{k^4}{\varepsilon^2} \nabla S \nabla S$$

- Validation

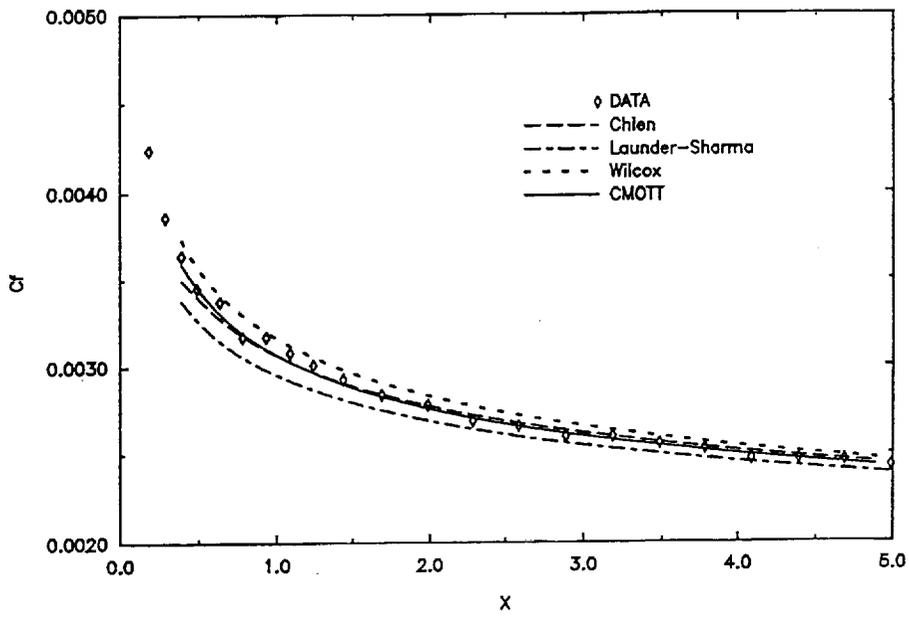
Flows:

- ◇ Channel flows
- ◇ Boundary layer flows with and without pressure gradients
- ◇ Planar jet, round jet and mixing layer
- ◇ Backward-facing step flows
- ◇ Complex flows related to industrial applications

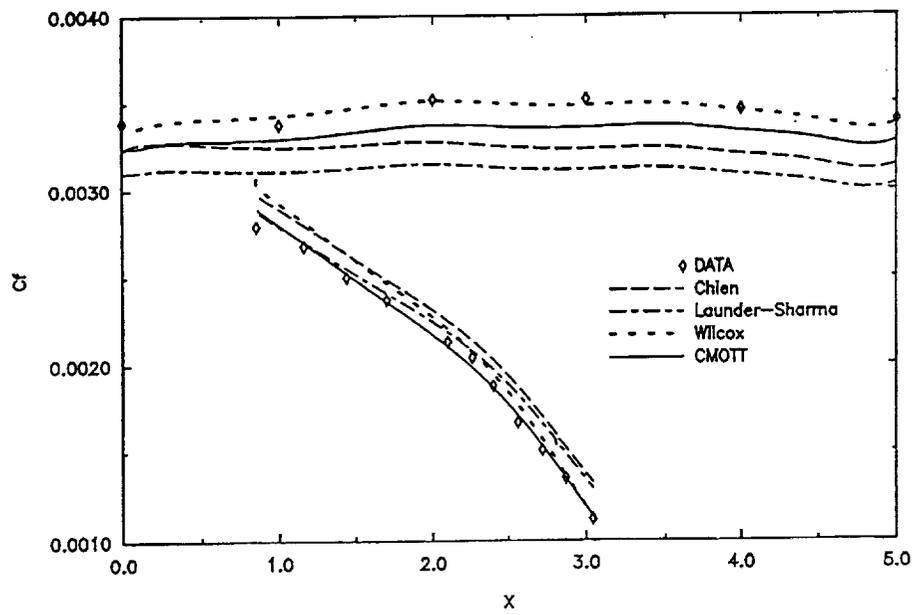
Models:

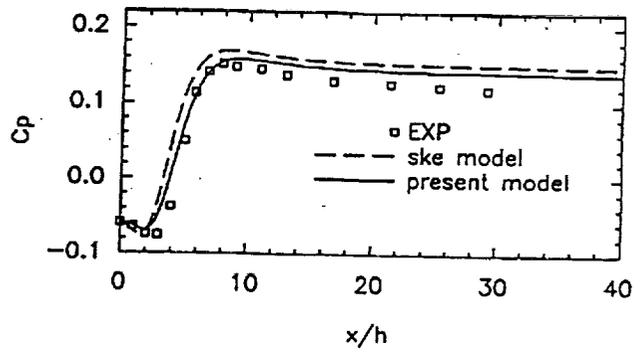
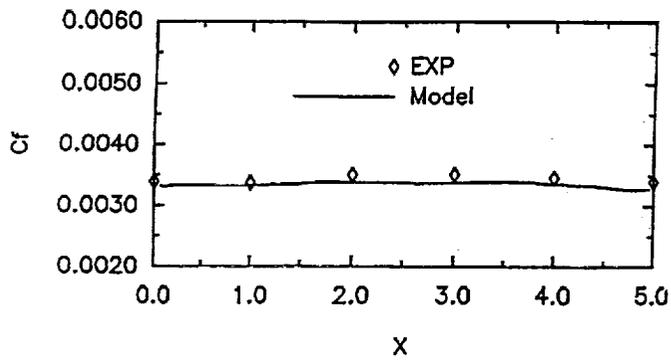
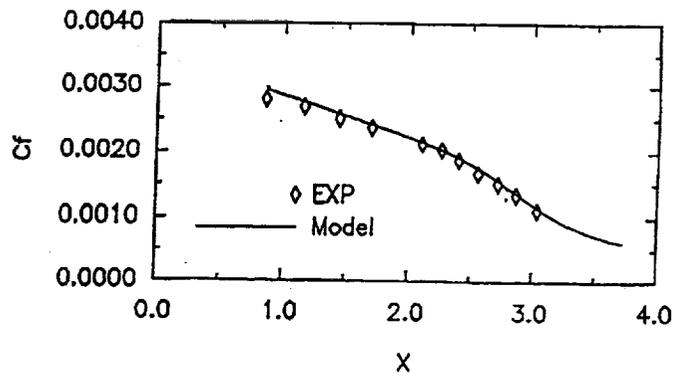
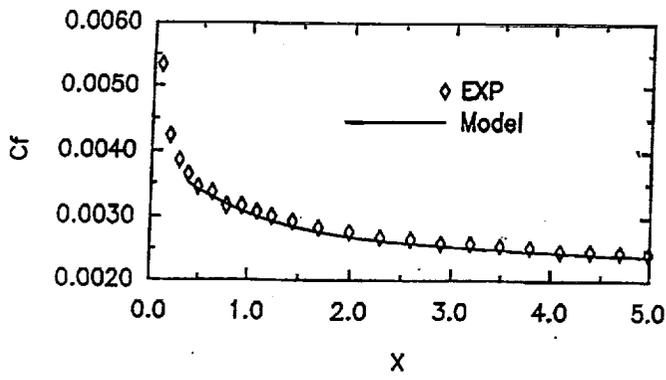
- ◇ Launder-Sharma, Lam-Bremhorst, Chien, Nagano-Hishida, ...
- ◇ $k - \omega$ model (Wilcox)
- ◇ CMOTT $k - \varepsilon$ model

Turbulent Boundary Layer



Turbulent Boundary Layer

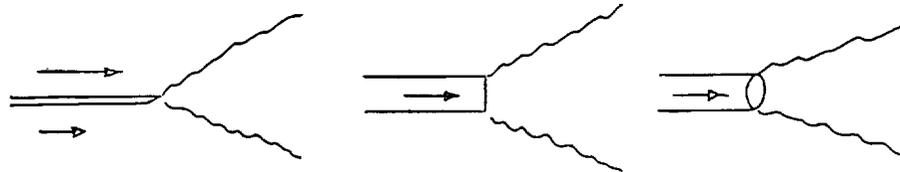




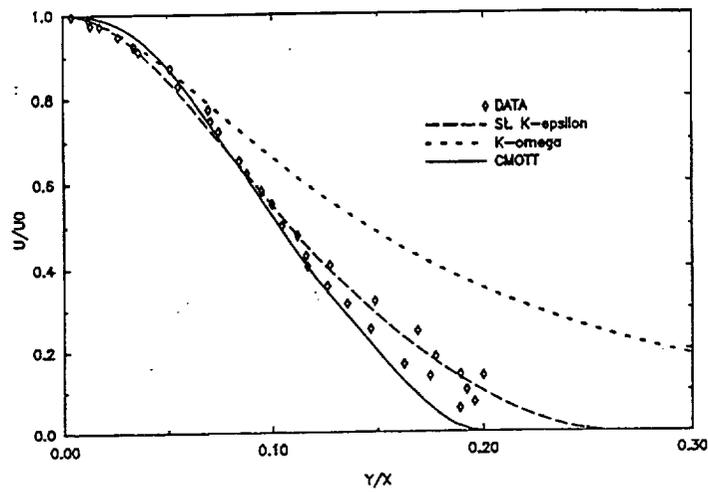
Present model with the modified wall function

Spreading Rate of Free Shear Flows

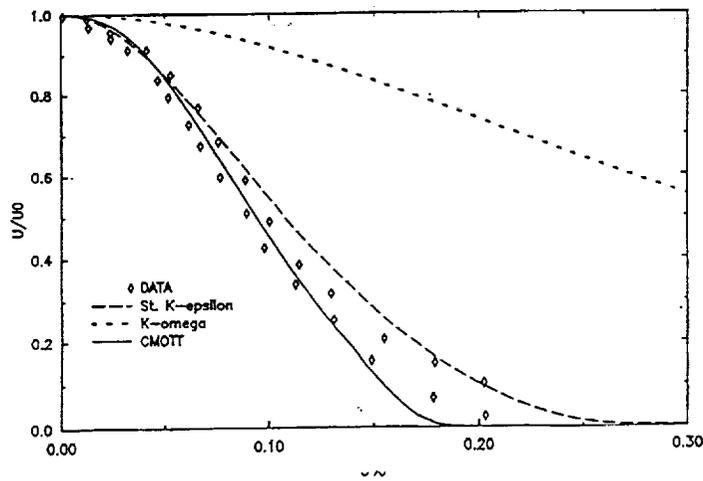
	exp.	st. $k - \epsilon$	Chien	$k - \omega$	CMOTT
Planar Jet	0.10-0.11	0.108	0.098	0.14*	0.102
Round Jet	0.085-0.095	0.116	0.104	0.32*	0.095
Mixing Layer	0.13-0.17	0.152	0.152	0.16*	0.154



Planar Jet



Round Jet



Algebraic Reynolds stress models

- Objective

- ◇ To examine the deficiencies of existing ARS models
- ◇ To develop better ARS models

- Current status of ARS models

- ◇ Second-order closure based ARS models (Rodi, 1980)

$$\frac{\overline{u_i u_j}}{k} (P - \varepsilon) = -\overline{u_i u_k} U_{j,k} - \overline{u_j u_k} U_{i,k} - \frac{1}{\rho} (\overline{p_{,i} u_j} + \overline{p_{,j} u_i}) - 2\nu \overline{u_{i,k} u_{j,k}}$$

Comments:

- * Assumption: $\overline{u_i u_j} / k = \text{Const.}$, $(\overline{u_i u_j u_k})_{,k} = (\overline{k u_i})_{,i} = 0$
- * Numerical difficulties
- ◇ Pope's explicit ARS model (2-D flows), Taulbee's ARS model (3-D), Gatski and Speziale's ARS model
- ◇ Other methods: RNG, DIA and invariant theory

- General constitutive relations from invariant theory

$$\begin{aligned}
\overline{u_i u_j} &= \frac{2}{3} k \delta_{ij} + 2a_2 \frac{K^2}{\varepsilon} (U_{i,j} + U_{j,i} - \frac{2}{3} U_{i,i} \delta_{ij}) + 2a_4 \frac{K^3}{\varepsilon^2} (U_{i,j}^2 + U_{j,i}^2 - \frac{2}{3} \Pi_1 \delta_{ij}) \\
&+ 2a_6 \frac{K^3}{\varepsilon^2} (U_{i,k} U_{j,k} - \frac{1}{3} \Pi_2 \delta_{ij}) + 2a_7 \frac{K^3}{\varepsilon^2} (U_{k,i} U_{k,j} - \frac{1}{3} \Pi_2 \delta_{ij}) \\
&+ 2a_8 \frac{K^4}{\varepsilon^3} (U_{i,k} U_{j,k}^2 + U_{i,k}^2 U_{j,k} - \frac{2}{3} \Pi_3 \delta_{ij}) + 2a_{10} \frac{K^4}{\varepsilon^3} (U_{k,i} U_{k,j}^2 + U_{k,j} U_{k,i}^2 - \frac{2}{3} \Pi_3 \delta_{ij}) \\
&+ 2a_{12} \frac{K^5}{\varepsilon^4} (U_{i,k}^2 U_{j,k}^2 - \frac{1}{3} \Pi_4 \delta_{ij}) + 2a_{13} \frac{K^5}{\varepsilon^4} (U_{k,i}^2 U_{k,j}^2 - \frac{1}{3} \Pi_4 \delta_{ij}) \\
&+ 2a_{14} \frac{K^5}{\varepsilon^4} (U_{i,k} U_{l,k} U_{l,j}^2 + U_{j,k} U_{l,k} U_{l,i}^2 - \frac{2}{3} \Pi_5 \delta_{ij}) \\
&+ 2a_{16} \frac{K^6}{\varepsilon^5} (U_{i,k} U_{l,k}^2 U_{l,j}^2 + U_{j,k} U_{l,k}^2 U_{l,i}^2 - \frac{2}{3} \Pi_6 \delta_{ij}) \\
&+ 2a_{18} \frac{K^7}{\varepsilon^6} (U_{i,k} U_{l,k} U_{l,m}^2 U_{j,m}^2 + U_{j,k} U_{l,k} U_{l,m}^2 U_{i,m}^2 - \frac{2}{3} \Pi_7 \delta_{ij})
\end{aligned}$$

- RDT and realizability constraints (Reynolds, Lumley)
- CMOTT algebraic Reynolds stress model

$$\overline{u_i u_j} = \frac{2}{3} k \delta_{ij} - C_\mu \frac{k^2}{\varepsilon} 2S_{ij}^* + 2C_2 \frac{k^3}{\varepsilon^2} (-S_{ik}^* \Omega_{kj}^* + \Omega_{ik}^* S_{kj}^*)$$

$$k_{,t} + U_j k_{,j} = [(\nu + \frac{\nu_t}{\sigma_k}) k_{,j}]_{,j} - \overline{u_i u_j} U_{i,j} - \varepsilon$$

$$\varepsilon_{,t} + U_j \varepsilon_{,j} = [(\nu + \frac{\nu_t}{\sigma_\varepsilon}) \varepsilon_{,j}]_{,j} - C_{e1} \frac{\varepsilon}{k} \overline{u_i u_j} U_{i,j} - C_{e2} \frac{\varepsilon^2}{k}$$

where

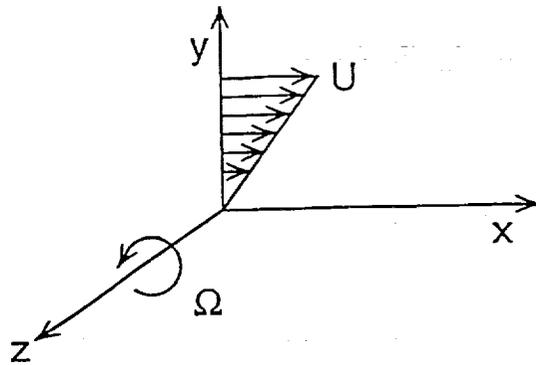
$$C_\mu = \frac{1}{A_0 + A_s^* \frac{U^* k}{\varepsilon}}, \quad C_2 = \frac{\sqrt{1 - 9C_\mu^2 (\frac{S^* k}{\varepsilon})^2}}{C_0 + 6 \frac{S^* k}{\varepsilon} \frac{\Omega^* k}{\varepsilon}}$$

$$\nu_t = C_\mu \frac{k^2}{\varepsilon}, \quad A_0 = 6.5, \quad C_0 = 1.0$$

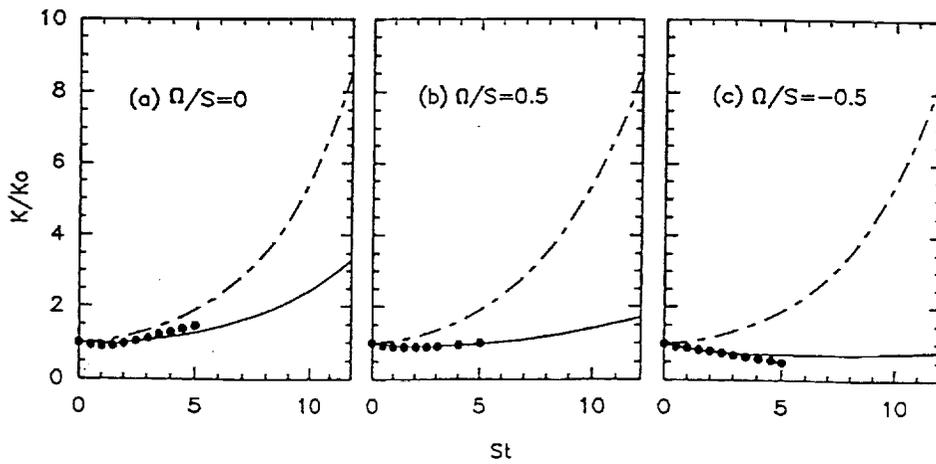
$$C_{e1} = 1.44, \quad C_{e2} = 1.92, \quad \sigma_k = 1, \quad \sigma_\varepsilon = 1.3$$

- Validation

- ◇ Rotating homogeneous shear flows
- ◇ Backward-facing step flows
- ◇ Confined jets
- ◇ Complex flows related to industrial applications



Configuration of rotating homogeneous shear flow



Evolution of turbulent kinetic energy with time.
 — : present model; - - - : SKE; • : LES

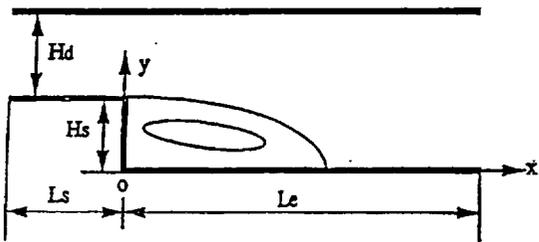
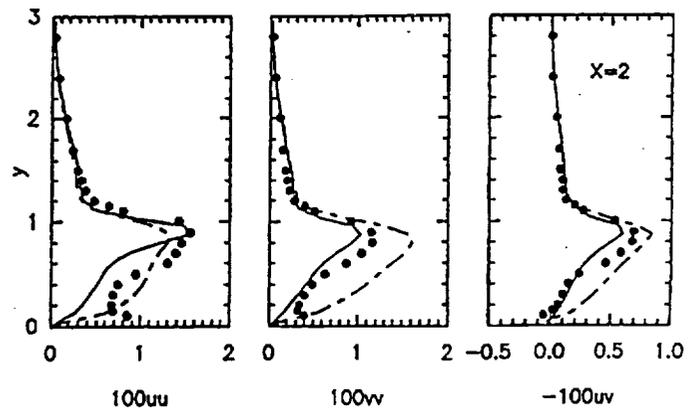
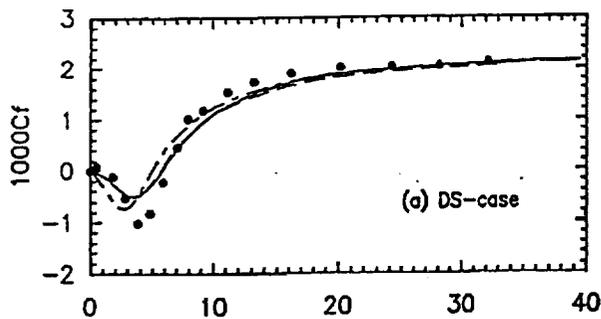
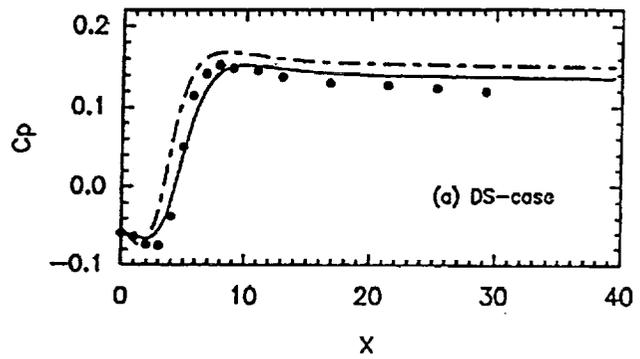
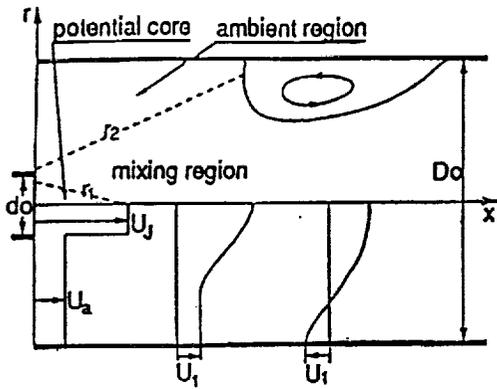


Table Comparison of the reattachment points

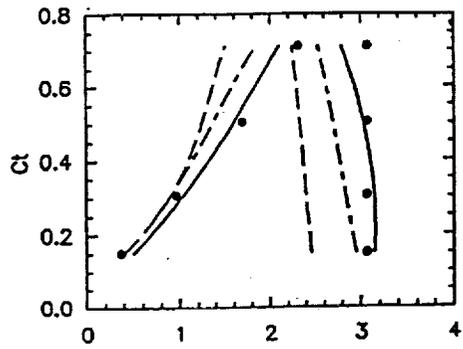
Case	measurement	SKE	PRESENT
DS	6.1	4.99	5.82
KKJ	7 ± 0.5	6.35	7.35



— : present model; - - - : SKE; • : EXP

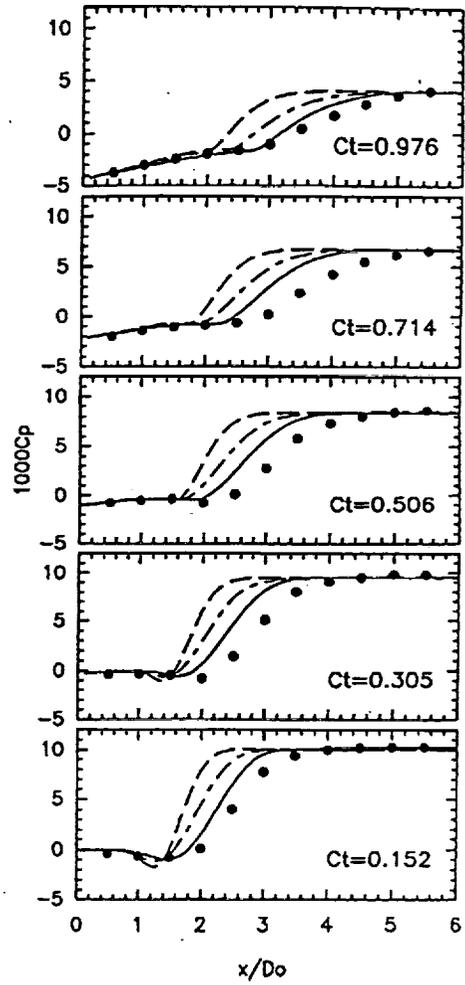


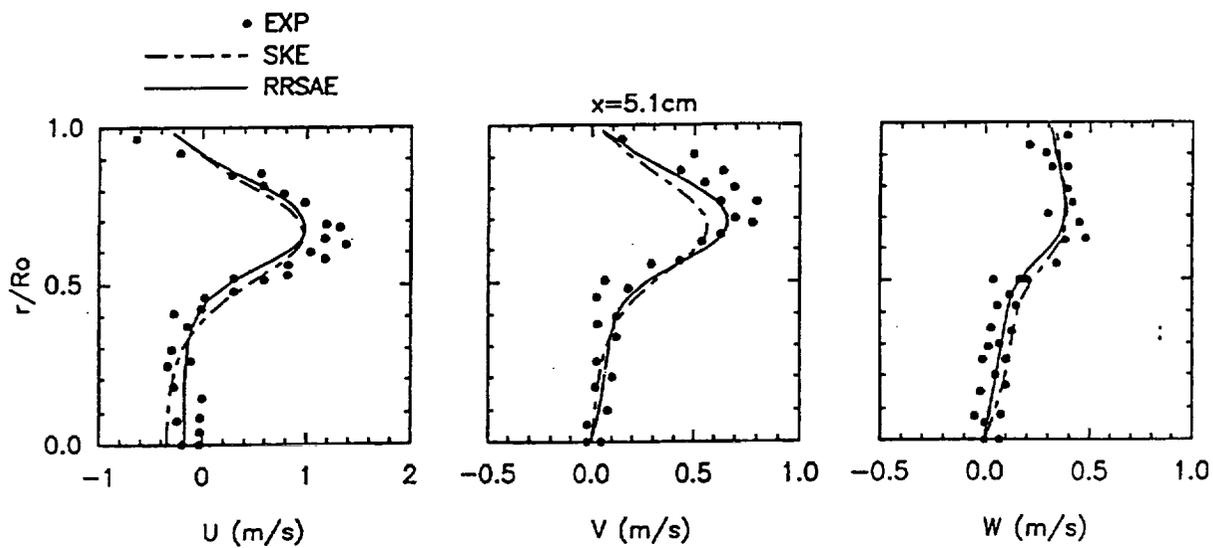
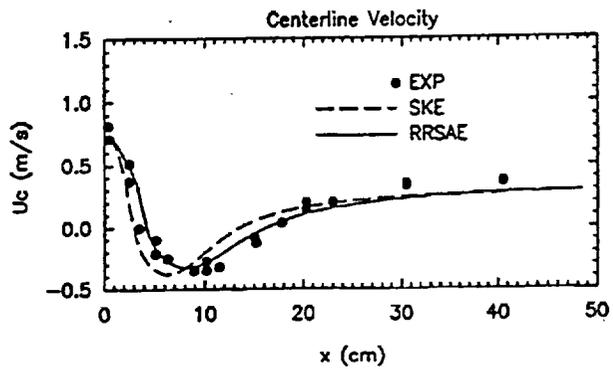
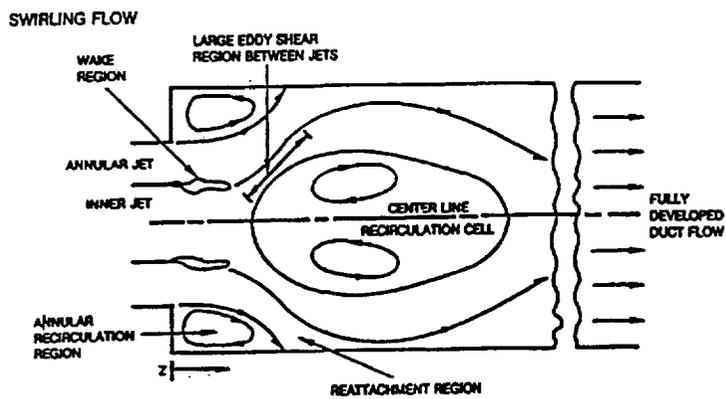
Flow configuration and notations



Separation and reattachment points

- EXP
- SKE
- - - RNG
- RRSAE





Scalar turbulence model

- Objective

To improve the predictive capability of current scalar turbulence ($\overline{\theta^2} - \epsilon_\theta$) models

- ◇ A new scalar flux constitutive relation
- ◇ A new scalar dissipation rate model equation

$$\overline{u_i \theta} = -C_\lambda \frac{k^2}{\epsilon} \left(\frac{2}{r}\right)^{1/2} \Theta_{,i} + \frac{k^3}{\epsilon^2} \left(\frac{2}{r}\right)^{1/2} (a_2 U_{i,j} + a_3 U_{j,i}) \Theta_{,j}$$

$$U_j \frac{\partial \overline{\theta^2}}{\partial x_j} = \left(\frac{\alpha_T}{\sigma_t} \overline{\theta^2}_{,j}\right)_{,j} - 2\overline{u_i \theta} \frac{\partial \Theta}{\partial x_i} - 2\epsilon_\theta$$

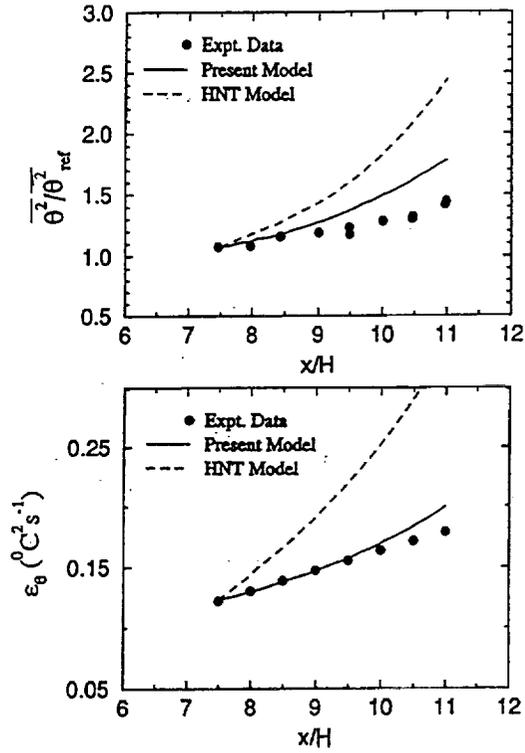
$$U_j \frac{\partial \epsilon_\theta}{\partial x_j} = \left(\frac{\alpha_T}{\sigma_\phi} \epsilon_{\theta,j}\right)_{,j} + C_{\theta 1} \epsilon_\theta S + C_{\theta 2} \sqrt{\frac{\epsilon_\theta \epsilon}{Pr}} S_T - C_{\theta 3} \frac{\epsilon_\theta \epsilon}{k}$$

$$C_\lambda = \frac{(2 + 2r + 0.5r^2)}{26 + 3.2\eta^2 + 2\xi^2}$$

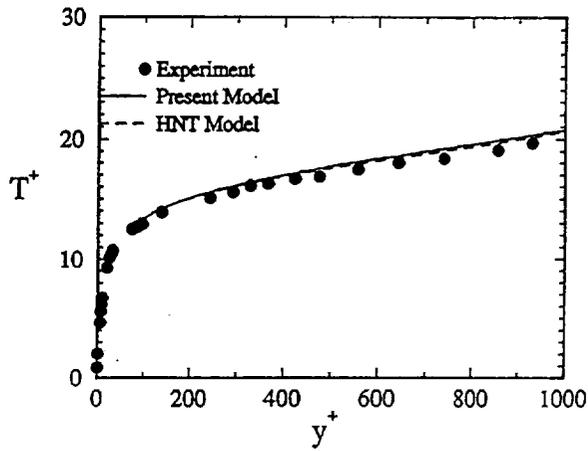
$$S_T = \sqrt{\Theta_{,i} \Theta_{,i}}, \quad S = \sqrt{2S_{ij} S_{ij}}, \quad \eta = Sk/\epsilon, \quad \xi = \frac{k}{\epsilon} \left(\frac{k}{\theta^2}\right)^{1/2} S_T, \quad r = \frac{2k}{\epsilon} \frac{\epsilon_\theta}{\theta^2}$$

$$C_{\theta 1} = C_1 - 0.13, \quad C_{\theta 2} = 0.63, \quad C_{\theta 3} = C_2 - 1, \quad \sigma_t = 1.0, \quad \sigma_\phi = 1.8$$

Tavoularis & Corrsin Expt (1981)



Flat plate boundary layer with constant surface temperature



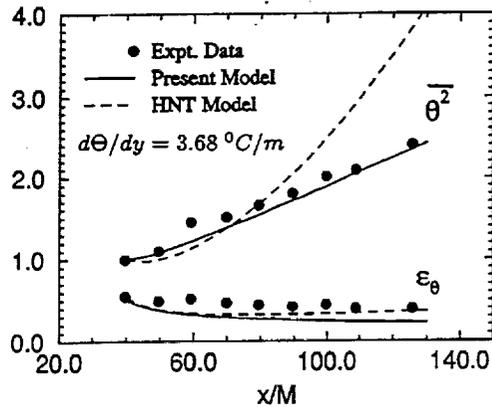
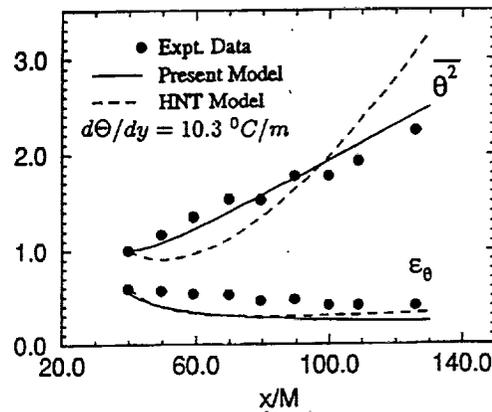
- Validation

- ◇ Homogeneous turbulence subjected to $\partial\Theta/\partial y$
- ◇ Homogeneous turbulence subjected to $\partial U/\partial y, \partial\Theta/\partial y$
- ◇ Flat plate boundary layer with constant surface temperature

- Work in progress

- ◇ Model assessment for different scalar boundary conditions
- ◇ Model extension for integration to the wall

Sirivat & Warhaft Expt (1983)



Second Order Closure Models

$$\frac{D\overline{u_i u_j}}{Dt} = T_{ij} + P_{ij} + \Pi_{ij}^{\text{Rapid}} + \Pi_{ij}^{\text{Return}} - \frac{2}{3}\varepsilon\delta_{ij}$$

- Objective

- ◇ To assess existing models
- ◇ To find the direction of improving closure models

- Basic model forms

$$\Pi_{ij}^{\text{Rapid}} = F_{ij}(S_{ij}, \overline{u_i u_j}),$$

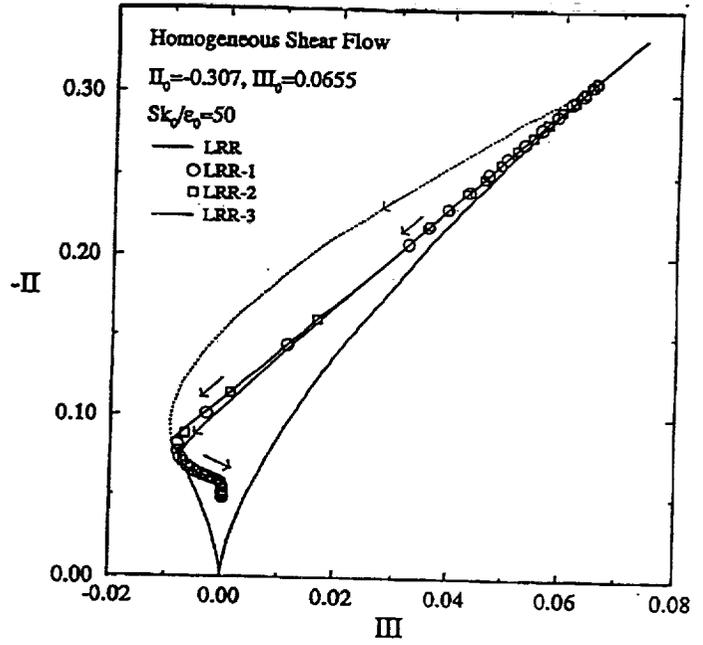
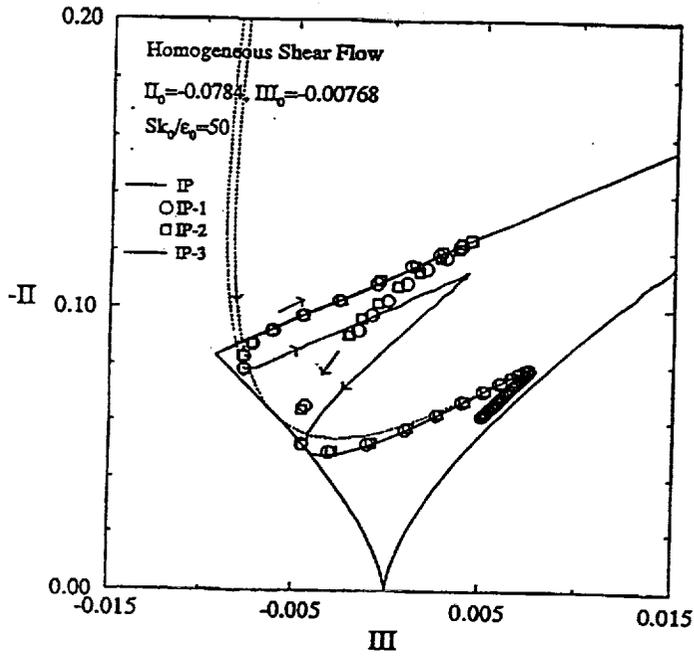
$$\Pi_{ij}^{\text{Return}} = F_{ij}(\overline{u_i u_j}, \nu, k, \varepsilon),$$

$$T_{ij} = F_{ij}((\overline{u_i u_j})_{,k}, k, \varepsilon)$$

- General comments on second order closures:

- ◇ The model, Π_{ij}^{Rapid} , is relatively well developed compared with other terms
- ◇ The model, Π_{ij}^{Return} , is least developed
- ◇ A Galilean and tensorially invariant second order closure model has not been well developed yet
- ◇ All models have large errors near the wall, especially in the buffer layer; therefore, for engineering application, the wall function approach is suggested at the present time

- Application of realizability to IP and LRR models



Multiple scale k - ϵ model

- **Objective:**

- ◇ To consider the effect of a non-equilibrium energy spectrum on eddy viscosity for compressible turbulence

- **Approach:**

- ◇ Use multiple scale concept introduced by

□ Large-Scale

$$\bar{\rho} \frac{\overline{D\tilde{k}_p}}{\overline{Dt}} = \frac{\partial}{\partial y} \left[\left(\bar{\mu} + \frac{\mu_T}{\sigma_{\tilde{k}_p}} \right) \frac{\partial \tilde{k}_p}{\partial y} \right] + \mu_T \left(\frac{\partial \tilde{u}}{\partial y} \right)^2 - \bar{\rho} \tilde{\epsilon}_p + \text{fc}_1$$

$$\bar{\rho} \frac{\overline{D\tilde{\epsilon}_p}}{\overline{Dt}} = \frac{\partial}{\partial y} \left[\left(\bar{\mu} + \frac{\mu_T}{\sigma_{\tilde{\epsilon}_p}} \right) \frac{\partial \tilde{\epsilon}_p}{\partial y} \right] + C_{p1} \frac{\tilde{\epsilon}_p}{\tilde{k}_p} \mu_T \left(\frac{\partial \tilde{u}}{\partial y} \right)^2 - C_{p2} \bar{\rho} \frac{\tilde{\epsilon}_p^2}{\tilde{k}_p} + \text{fc}_2$$

- fc_1 - exchanges between the turbulent kinetic energy and internal energy
- fc_2 - increased spectral energy transfer due to compressibility effects

□ Small Scale

$$\bar{\rho} \frac{\overline{D\tilde{k}_t}}{\overline{Dt}} = \frac{\partial}{\partial y} \left[\left(\bar{\mu} + \frac{\mu_T}{\sigma_{\tilde{k}_t}} \right) \frac{\partial \tilde{k}_t}{\partial y} \right] + \bar{\rho} \tilde{\epsilon}_p - \bar{\rho} \tilde{\epsilon}_t$$

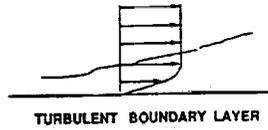
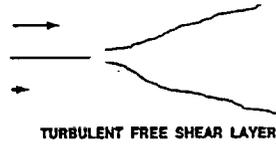
$$\bar{\rho} \frac{\overline{D\tilde{\epsilon}_t}}{\overline{Dt}} = \frac{\partial}{\partial y} \left[\left(\bar{\mu} + \frac{\mu_T}{\sigma_{\tilde{\epsilon}_t}} \right) \frac{\partial \tilde{\epsilon}_t}{\partial y} \right] + C_{t1} \bar{\rho} \frac{\tilde{\epsilon}_t \tilde{\epsilon}_p}{\tilde{k}_t} - C_{t2} \bar{\rho} \frac{\tilde{\epsilon}_t^2}{\tilde{k}_t}$$

□ Eddy Viscosity

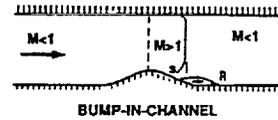
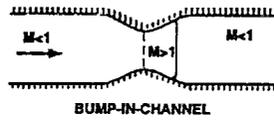
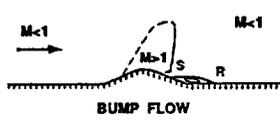
$$\mu_T \approx \bar{\rho} u l \approx \bar{\rho} (\tilde{k}_p + \tilde{k}_t)^{\frac{1}{2}} \frac{(\tilde{k}_p + \tilde{k}_t)^{\frac{3}{2}}}{\tilde{\epsilon}_p}$$

Model Evaluation

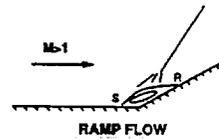
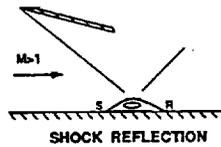
- Turbulent Shear Flow



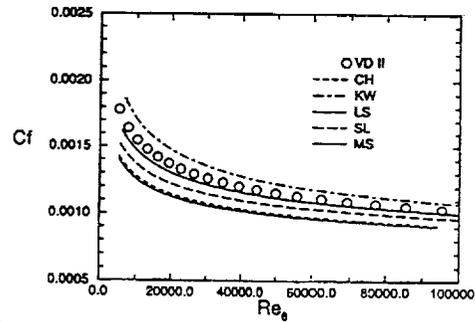
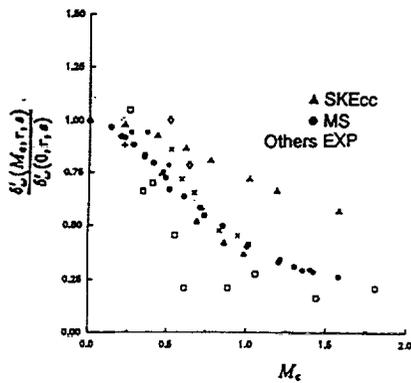
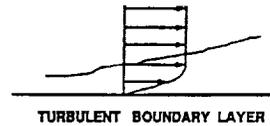
- Shock/Turbulent-Boundary-Layer Interactions
 - ◇ transonic flow



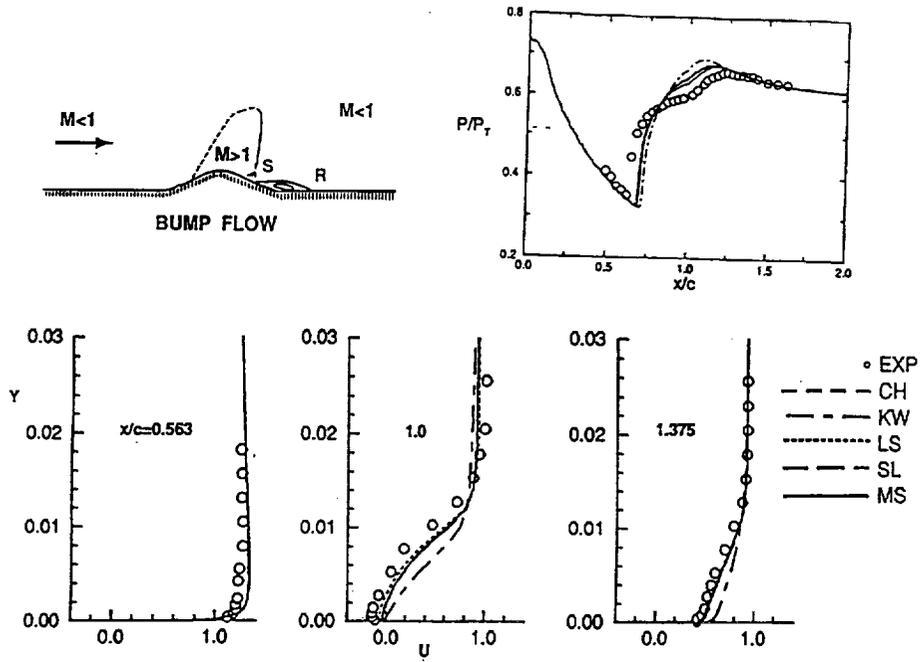
- ◇ supersonic flow



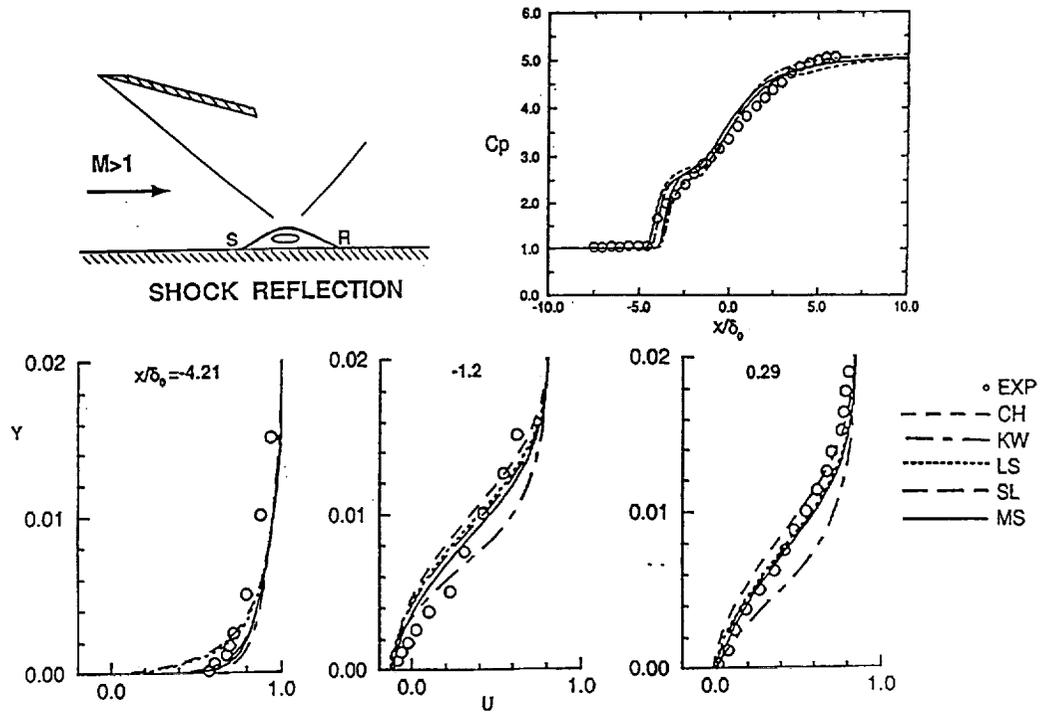
Compressible Turbulent Shear Flow



Flow over a Bump—Bachalo and Johnson (1979)



Shock Reflection—Reda *et. al* (1973-1977)



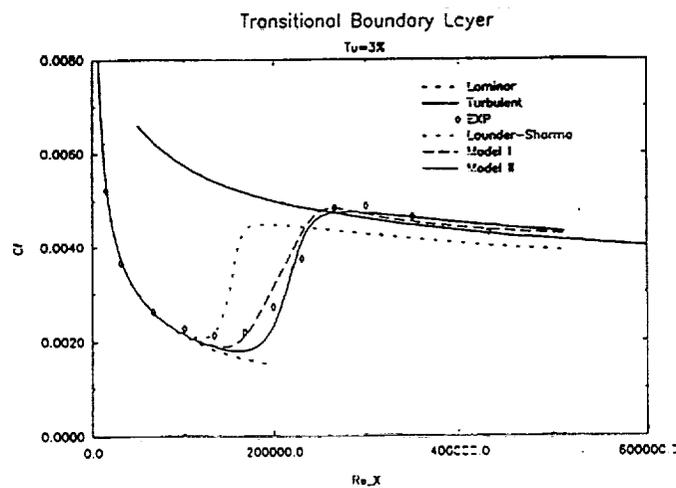
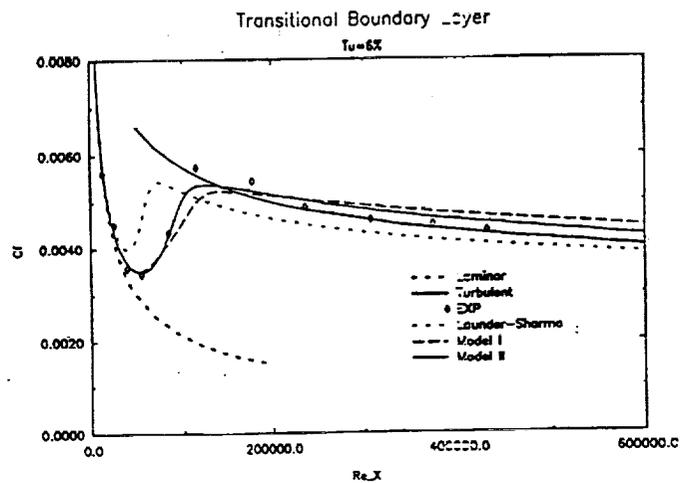
Bypass transition models

- Objective:

- ◊ Develop transition models for flows with free stream turbulence

- Approach:

- ◊ Using $K-\epsilon$ model as the base model
- ◊ Introduce effective intermittency to either the eddy viscosity or the $k-\epsilon$ model equations



PDF modeling of turbulent reacting flows

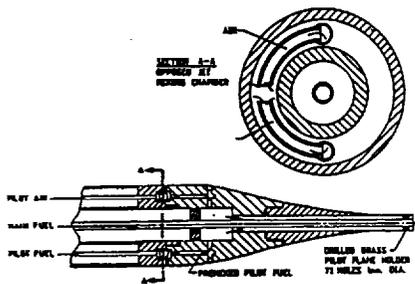
- Objective:

- ◇ Develop models that can accurately simulate finite chemical reactions in turbulent flows.
- ◇ Develop and validate independent PDF models.
- ◇ Technology transfer.

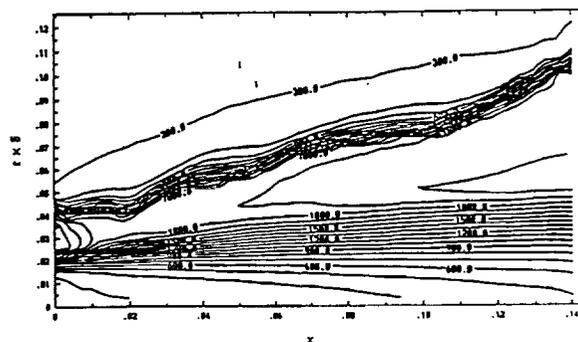
- Approach:

- ◇ Joint pdf for scalar compositions.
- ◇ Moment closure schemes for velocity field.
- ◇ Develop hybrid solver consisting of Monte Carlo method and finite-difference/finite-volume method.

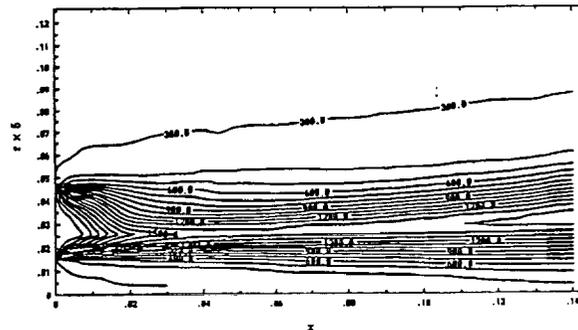
BURNER JET



Without PDF Method



With PDF Method. (CMOTT)



Brian R. Smith
CFD Group
Lockheed Fort Worth Company
Fort Worth, Texas

Broad Range of Flow Problems of Interest

Wide Range of Flow Conditions:

Subsonic – Hypersonic
Internal – External – Store Separation
Cruise – High Angle of Attack

Flows phenomena of interest:

Inlets/Diffusers

Streamwise Curvature
Shock/BL Interactions
Rectangular Duct → Circular

Leading Edge Separation – Cowl Lips
Separation Induced Unstart

Nozzles

Entrainment
Round → Rectangular Duct
High Speed Shear Layers

Film cooling, Liners, Vanes
Swirl

External Aerodynamics

Vortex
Leading Edge Separation
Shock/BL Interactions

3D Boundary Layers
Wakes

The CFD Environment at Lockheed Fort Worth Company

- Most codes developed or highly modified in house
- General grid generation and solvers for diverse applications
- Structured and unstructured solvers
- Computational efficiency important
 - Complex geometries, many gridpoints
 - Large arrays of flow conditions

Requirements for Turbulence Models

Turbulence Modeling Priorities for Industrial Application

- Validation
 - High accuracy for attached flows
 - Reasonable accuracy for all flows
 - High confidence level
- Computational efficiency
- Robust for complex geometries
- Transitional modeling capability

To obtain acceptable accuracy, propulsion flows demand more sophisticated turbulence models than do external aerodynamic flows

The $k - k_l$ and $k - l$ Two Equation Turbulence Models

Advantages of using k_l or l instead of ϵ or ω

k_l and l equations are easier to resolve numerically than ϵ equation

Dissipation Length Scale is an integral length scale

- Can derive equation for volume integral of two point correlation function.
- Theoretical ϵ equation is dominated by small scales

$k - k_l$ and $k - l$ agree better with compressible boundary layer data than does $k - \epsilon$

Disadvantage - current formulation requires calculation of distance to walls

$k - k_l$ model

- Includes unique, consistent wall function
- Accurate for transonic flows

$k - l$ model

- Derived from $k - k_l$ model - identical in high Re turbulence
- Near wall model simulates k in viscous sublayer

The k – ϵ Model Wall Function

Wall layer model derived from and consistent with the k – ϵ model

- Assume convection in momentum, energy and turbulent kinetic energy equations to be negligible
- Boundary layer approximation

Match velocity, k and ϵ at first grid point in Navier – Stokes solution

First grid point can be in viscous sublayer, buffer or logarithmic region

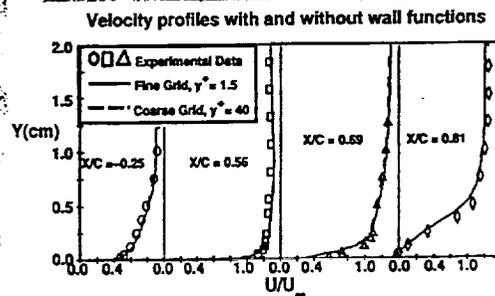
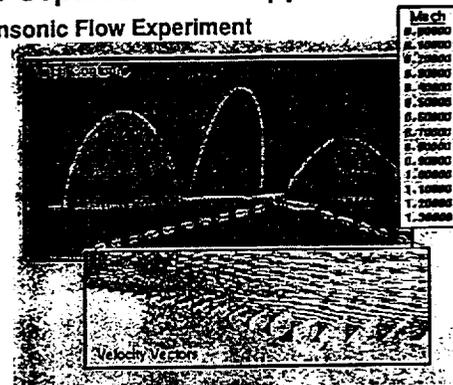
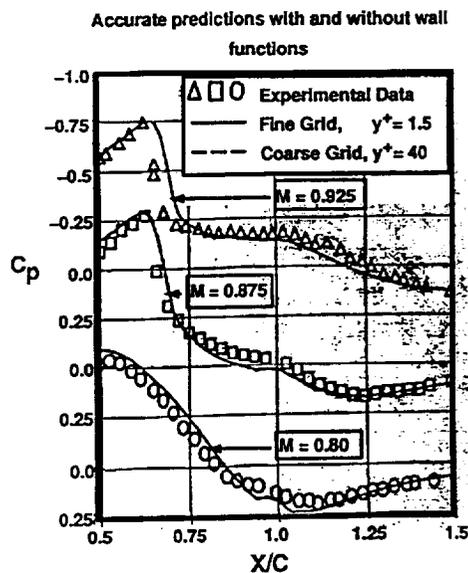
Boundary conditions on k and ϵ simple for k – ϵ model

Advantages of wall functions

- Reduces number of necessary grid points
- Reduces number of iterations to converge steady state solution 60 – 90%

Wall Functions are Accurate for Separated Flow Applications

Axisymmetric Bump, Transonic Flow Experiment



The k - I Model with Near Wall Model

kI equation is transformed exactly to an I equation

Advantages of k - I formulation

- I is linear near wall, kI nonlinear and very small
- Near wall damping terms disappear
- Production term drops out with current choice of constants

k - I model includes:

- Transitional flow modeling
- Compressibility corrections

Modeling of details of k profile near wall important for hypersonic flows

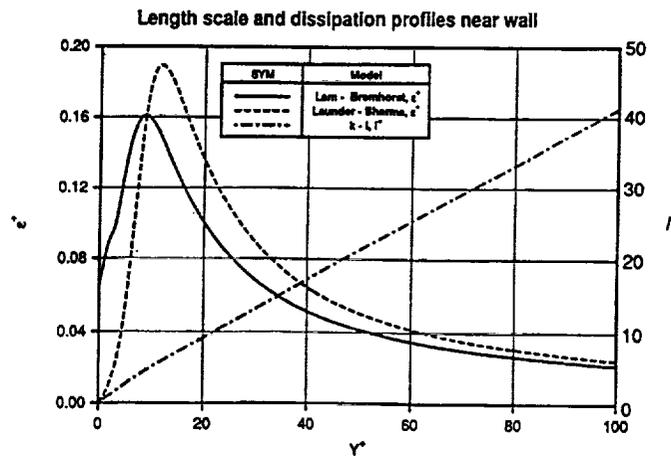
- Magnitude of normal stress term comparable to static pressure
- Near wall density variations large

I Equation Much Easier to Resolve than ϵ Equation

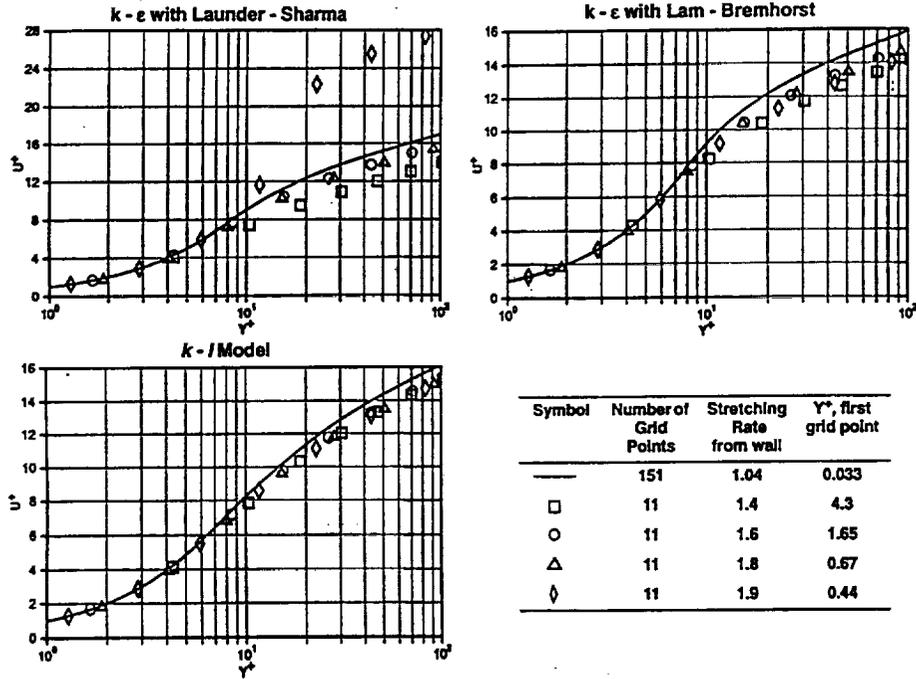
ϵ equation requires fine grid from wall to y^+ of 20 to resolve peak

- Exclusion of near wall viscous dissipation term aggravates problem
- Logarithmic region, $\epsilon \propto 1/y$

I equation is nearly linear near wall - much less sensitive to grid resolution



Resolution Study with $k - \epsilon$ and $k - l$ Models



Sample Applications:

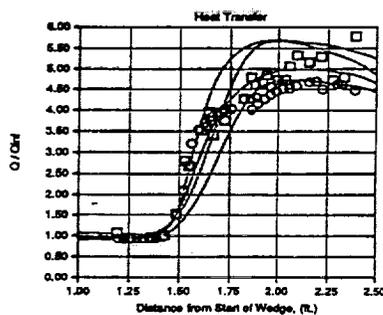
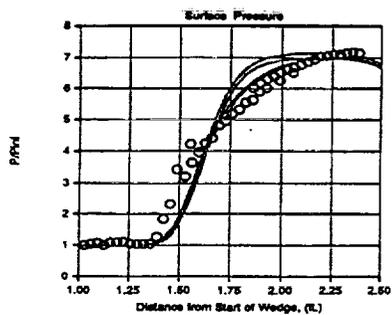
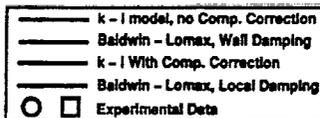
Mach 8 Shock Wave Turbulent Boundary Layer Interactions

F-16 Inlet Derivative, Isolated Duct Study

Multi-slot Ejector

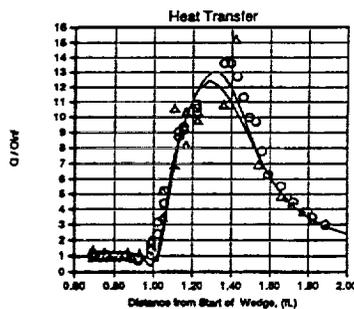
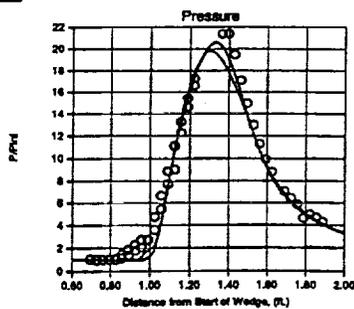
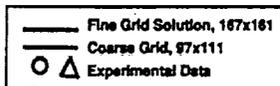
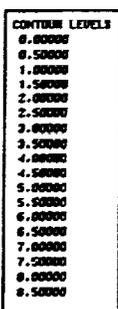
F110 Nozzle Drag Reduction Study

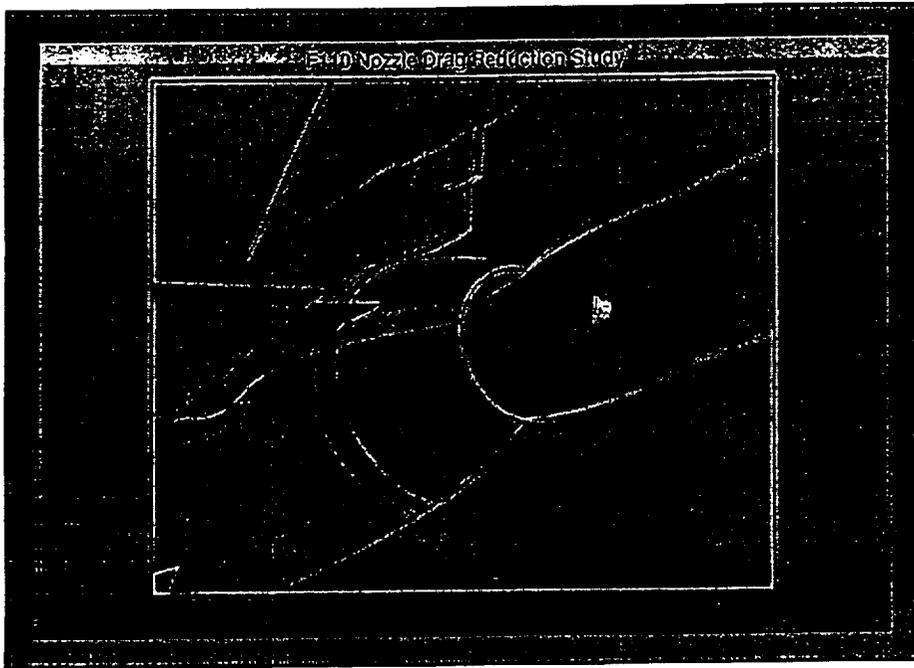
k - I Model With Compressibility Correction gives Best Prediction For Mach 8 Shock Boundary Layer Interaction



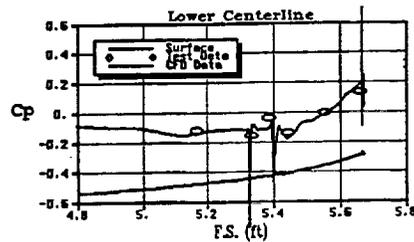
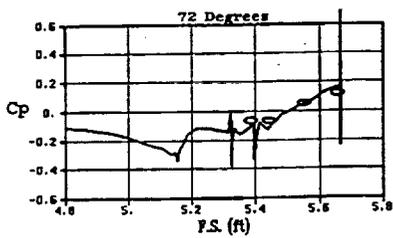
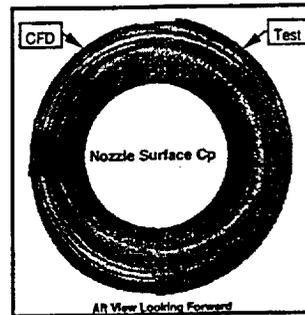
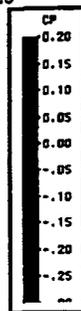
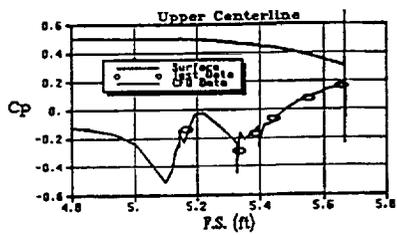
The k - I Model Predicts Turbulent Shock - Wave Boundary Layer Interaction Well

**Mach 8, 10 Degree Wedge Generator
2D case, Separated Flow**

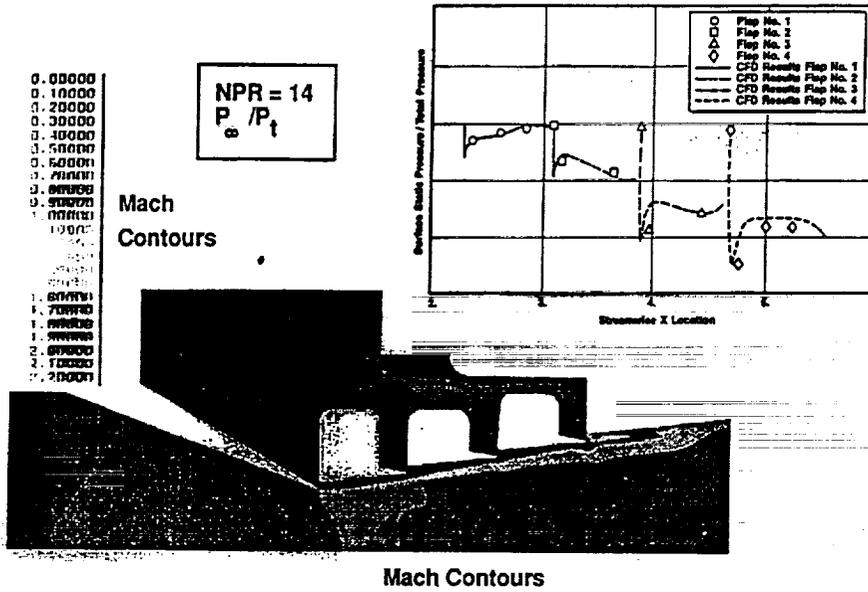




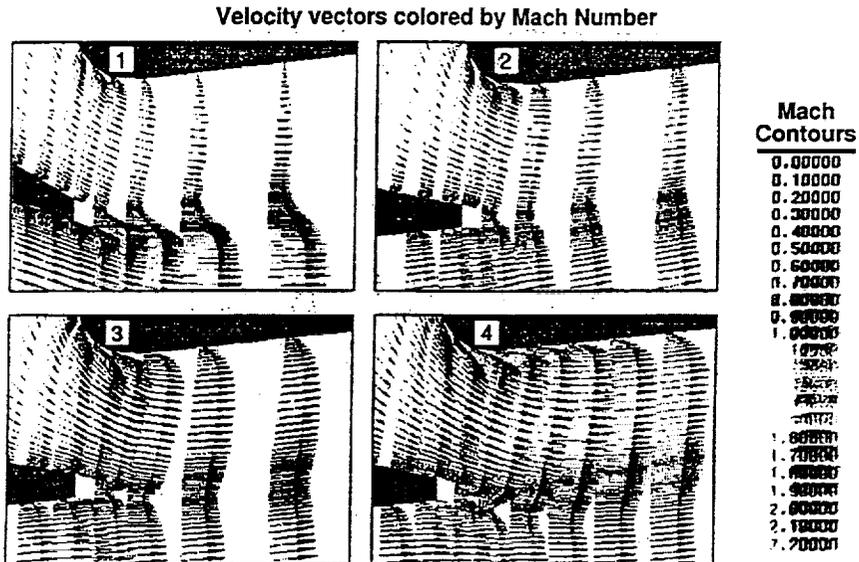
Afterbody/Nozzle Pressure Distributions Match Test Data
Mach 0.6



Good Predictions of Multi – Slot Ejector Obtained with k – kl Model



k – kl Model Predicts Entrainment Effects Near Slots



Summary

Computationally efficient k – l and k – kl models have been developed and implemented at Lockheed Fort Worth Company

Many years of experience applying two equation turbulence models to complex 3D flows for design and analysis

A SUMMARY OF COMPUTATIONAL EXPERIENCE AT GE AIRCRAFT ENGINES FOR
COMPLEX TURBULENT FLOWS IN GAS TURBINES

N95- 27885

R. Zerkle and C. Prakash
GE Aircraft Engines
Cincinnati, Ohio

CONTENTS:

- INTRODUCTION
- 2-D BOUNDARY LAYER CODE WITH LRN TURBULENCE MODEL
- 3-D NAVIER-STOKES CODE WITH WALL FUNCTIONS
- 3-D NAVIER-STOKES CODE WITH LRN TURBULENCE MODEL
- FILM COOLING SIMULATION
- TURBULATED PASSAGE SIMULATION
- OVERALL CONCLUSIONS
- LIST OF REFERENCES

INTRODUCTION:

- Indications are that the standard $k-\epsilon$ turbulence model together with standard wall functions are adequate for CFD simulations in cavities away from the primary gaspath of a gas turbine engine.
- However, CFD simulations in the primary gaspath and in blade cooling passages require more advanced turbulence models.
- Therefore, this presentation will summarize some CFD experience at GEAE only for flows in the primary gaspath of a gas turbine engine and in turbine blade cooling passages.

2-D BOUNDARY LAYER CODE WITH LOW REYNOLDS NUMBER (LRN) TURBULENCE MODEL:

- The STAN5 B.L. code was modified to include the LRN $k-\epsilon$ turbulence model of Lam & Bremhorst as described by Zerkle & Lounsbury [1].
- Includes the following near-wall effects:
 - High freestream turbulence
 - Axial pressure gradient
 - Onset of transition
 - Relaminarization
 - Wall roughness
 - Wall curvature
- Used to compute heat transfer coefficient distributions on turbine airfoil external surfaces.
- Primary limitation:
 - It's a 2-D code in a 3-D environment.

3-D NAVIER-STOKES CODE WITH WALL FUNCTIONS:

- Time-marching finite-volume formulation of the Reynolds-averaged Navier-Stokes equations as described by Turner & Jennions [2,3].
- Includes:
 - Explicit Runga-Kutta flow solver
 - Implicit formulation of the standard $k-\epsilon$ turbulence model
 - Standard wall functions
 - Transonic flow effects
- Used to simulate high speed flows in turbomachinery passages.
- Limitations:
 - Lacks near-wall physics of the 2-D boundary layer code.
 - For example, lack of boundary layer transition leads to overprediction of loss for some turbomachinery airfoil passages containing significant regions of transitional flow.

3-D NAVIER-STOKES CODE WITH LOW REYNOLDS NUMBER (LRN) TURBULENCE MODEL:

- The LRN $k-\epsilon$ turbulence model of Lam & Bremhorst was implemented in the 3-D Navier-Stokes code as described by Dailey, Jennions and Orkwis [4].
- Addition of the LRN turbulence model improved the prediction of loss for transitional flows.
- Primary limitation:
 - The need for a very fine grid in the near-wall region leads to excessive run times which renders the code impractical for design applications at this time.

FILM COOLING SIMULATION:

- Film cooling at the surface of an HP turbine airfoil is crucial to its life.
- Improvement of the film cooling process would significantly improve turbine performance by reducing the need for cooling air flow.
- CFD simulation could facilitate film cooling development by reducing the need for expensive cascade testing and, more importantly, by giving greater insight into the associated flow physics.
- A CFD simulation of film-cooling tests, which were carried out at the Univ. of Texas by Professors Crawford & Bogard, and their students, is described by Leylek & Zerkle [5].
- These tests are of special interest because the ranges of film cooling parameters are consistent with those typically found in gas turbine airfoil applications.
- The objective was to validate a CFD model of film cooling by comparing numerical and experimental results.

FILM COOLING SIMULATION (CONT'D):

- The model includes:
 - A 3-D, fully-elliptic, Navier-Stokes solution of the coupled flow in the plenum, film hole, and cross-stream regions.
 - An exact representation of the inclined, round, film-hole geometry using a highly-orthogonalized fine grid mesh.
 - The standard $k-\epsilon$ turbulence model with standard wall functions.

FILM COOLING SIMULATION (CONT'D):

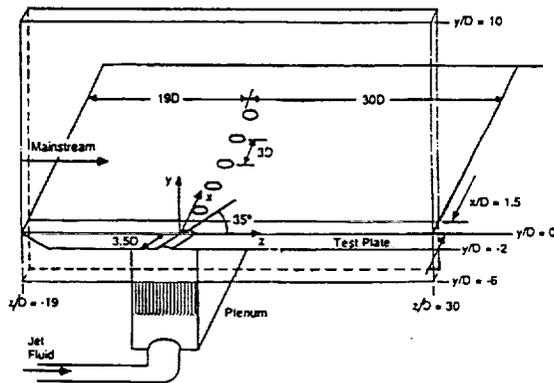


Figure 1. Essential features of experimental film cooling configuration showing overall extent of computation domain and coordinate system.

FILM COOLING SIMULATION (CONT'D):

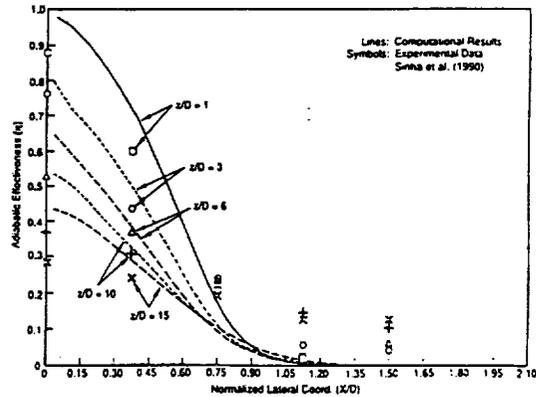


Figure 14 . Lateral variation of adiabatic effectiveness from computations and experiments for $M=0.5$ at five streamwise stations.

FILM COOLING SIMULATION (CONT'D):

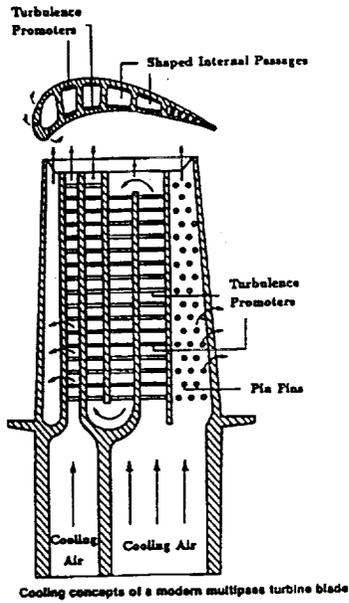
- Summary of Results:
 - The flowfield is dominated by a strong three-way coupling between the plenum, film-hole, and cross-stream regions.
 - Flow within the film hole is extremely complex, with counter-rotating vortices and local jetting effects.
 - A comparison of computed and experimental film effectiveness on the plate surface indicates that the simulated coolant jet is not spreading as fast as experimental results.
- Conclusions:
 - There is excellent *qualitative* agreement between the numerical and experimental results.
 - However, the lack of lateral spreading of the coolant is caused by the inability of the $k-\epsilon$ turbulence model to cope with non-uniform rates of diffusion in different directions.
 - Improved accuracy requires an *anisotropic* turbulence model.

TURBULATED PASSAGE SIMULATION:

- Modern high-performance turbine blades are cooled by internal radially-rotating serpentine passages.
- The air flowing through these passages is exposed to very large Coriolis and centripetal body forces which induce strong secondary flows and buoyant effects.
- These effects tend to increase heat transfer coefficient on the trailing face of an up-pass, but decrease it on the leading face.
- Turbulators are added to the passage walls in order to enhance their cooling effectiveness.
- The primary objective of blade cooling development is to determine turbulator and passage configurations which can influence the secondary flows to achieve a uniformly high heat transfer coefficient, but within pressure-drop constraints.
- Rotating-passage rig tests are expensive, and it is very difficult to achieve high-quality data in the range of engine operating parameters.

TURBULATED PASSAGE SIMULATION (CONT'D):

- Therefore, CFD could facilitate blade cooling development by simulating new cooling configurations at real engine operating conditions.
- An exploratory investigation of CFD simulation in turbulated blade cooling passages is described by Prakash & Zerkle [6].
- Conclusions are:
 - The flow fields in turbulated blade cooling passages are very complex, and desired accuracy requires advanced turbulence models.
 - An LRN model is needed near turbulated walls in the case of low passage Reynolds number.
 - An anisotropic turbulent model is needed in the case of large blockage ratio (rib height to passage diameter).
 - Practical LRN and anisotropic models are not yet available.



Blockage Ratio \rightleftarrows
Anisotropic and Multiple Length Scale Effects \rightleftarrows

	Low Blockage Ratio	High Blockage Ratio
Low Reynolds Number	<ul style="list-style-type: none"> • Need a low Reynolds number model • May not need a Reynolds stress model; i.e. an isotropic model may suffice 	<ul style="list-style-type: none"> • Need a low Reynolds number model • May need a Reynolds stress model <p style="text-align: center;"><i>Military Engines (Small)</i></p>
High Reynolds Number	<ul style="list-style-type: none"> • May not need a low Re model • May not need a Reynolds stress model; i.e. an isotropic model may suffice <p style="text-align: center;"><i>Commercial Engines</i></p>	<ul style="list-style-type: none"> • May not need a low Re model • May need a Reynolds stress model <p style="text-align: center;"><i>Large Commercial Engines</i></p>

Need for a Low Reynolds Number Model \updownarrow

Reynolds Number \updownarrow

Present Computations:
k- ϵ Model (Isotropic) with
Wall Functions

OVERALL CONCLUSIONS:

- Application of the standard $k-\epsilon$ turbulence model with wall function is not adequate for accurate CFD simulation of aerodynamic performance and heat transfer in the primary gas path of a gas turbine engine
- New models are required in the near-wall region which include more physics than wall functions. The two-layer modeling approach appears attractive because of its computational economy.
- In addition, improved CFD simulation of film cooling and turbine blade internal cooling passages will require anisotropic turbulence models
- New turbulence models must be practical in order to have a significant impact on the engine design process.
- A coordinated turbulence modeling effort between NASA center would be beneficial to the gas turbine industry.

LIST OF REFERENCES:

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2. Turner, M. G., and Jennions, I. K., 1993, "An Investigation of Turbulence Modeling in Transonic Fans Including a Novel Implementation of an Implicit $k-\epsilon$ Turbulence Model," *ASME Journal of Turbomachinery*, Vol. 115, pp. 249-260.
3. Jennions, I. K., and Turner, M. G., 1993, "3-D Navier-Stokes Computations of Transonic Fan Flow Using an Explicit Flow Solver and an Implicit $k-\epsilon$ Solver," *ASME Journal of Turbomachinery*, Vol. 115, pp. 261-272.
4. Dailey, L. D., Jennions, I. K., and Orkwis, P. D., 1994, "Simulating Laminar-Turbulent Transition With a Low Reynolds Number $k-\epsilon$ Turbulence Model in a Navier-Stokes Flow Solver," *AIAA Paper 94-0189*.
5. Leylek, J. H., and Zerkle, R. D., 1994, "Discrete-Jet Film Cooling: A Comparison of Computational Results With Experiments," *ASME Journal of Turbomachinery*, Vol. 116, pp. 358-368.
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THE APPLICABILITY OF TURBULENCE MODELS TO AERODYNAMIC AND PROPULSION
FLOWFIELDS AT McDONNELL DOUGLAS AEROSPACE

N95- 27886

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Objective

- Evaluate turbulence models for integrated aircraft components such as the forebody, wing, inlet, diffuser, nozzle, and afterbody

Approach

- Integrate turbulence models into existing Navier–Stokes program maintaining zonal philosophy
- Introduce corrections to baseline turbulence models to account for additional affects such as compressibility or separation
- Develop algorithmic improvements for better numerical stability and robustness
- Compare the strengths and weaknesses of turbulence models
- Determine applicability of algebraic, one–equation, and two–equation turbulence models for typical complex flows and geometries

Turbulence Modeling Capabilities

- *Algebraic Models*
 - Cebeci-Smith boundary layer model
 - Baldwin-Lomax boundary layer model
 - P. D. Thomas shear layer model
- *One-Equation Models*
 - Baldwin-Barth
 - Spalart-Allmaras
- *Two-Equation Models*
 - High Reynolds number $k - \epsilon$
 - Low Reynolds number $k - \epsilon$ (Jones-Launder, Speziale, Chien, Lam-Bremhorst, So, and Huang-Coakley)
 - Wilcox $k - \omega$
 - Menter baseline and shear-stress transport blended $k - \omega/k - \epsilon$

Navier-Stokes Time-Dependent Algorithm NASTD

- *Euler/Navier-Stokes Equations*
 - Laminar or Turbulent
 - Ideal Gas, Thermally Perfect Air, Equilibrium or Nonequilibrium Chemistry
- *Finite Volume Formulation*
 - Roe and Coakley Flux Difference Split Schemes, Optional TVD Schemes
- *Solution Update Procedure*
 - Approximate Factorization
 - Runge-Kutta Time Stepping
 - Iterative Space Marching (PNS)
- *Geometric Capabilities/Generalizations*
 - Zonal Capabilities and Flexible Boundary Conditions
 - Grid Sequencing
 - Overlapping Grids
- *Turbulence Models*
 - Cebeci-Smith, Baldwin-Lomax and P. D. Thomas Algebraic Models
 - Baldwin-Barth and Spalart Allmaras One-Equation Models
 - Six Low Reynolds Number $k - \epsilon$ Models
 - $k - \omega$ and Menter blended $k - \omega/k - \epsilon$ Models

Selected Applications

- Transonic Supercritical Airfoil
- Three-Element High-Lift System
- Single Slot 2-D Ejector Nozzle
- Confluent Mixer
- Highly Offset 3-D Diffuser

Modifications to Production Term

Default calculation of production:

$$P_k = \frac{\bar{\mu}_t}{Re} \left[\frac{1}{2} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)^2 - \frac{2}{3} \left(\frac{\partial \tilde{u}_k}{\partial x_k} \right)^2 \right] - \frac{2}{3} \bar{\rho} k \frac{\partial \tilde{u}_k}{\partial x_k}$$

Vorticity used in production:

$$P_k^* = \frac{\bar{\mu}_t}{Re} |\omega|^2$$

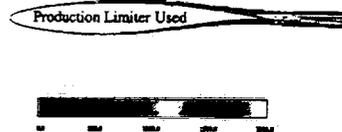
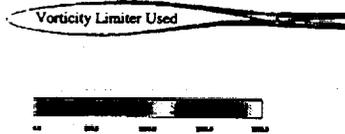
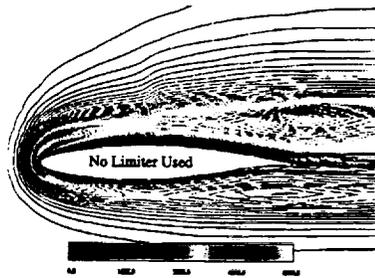
Production limiter used:

$$P_k^* = \min(P_k, 20D_k) = \min(P_k, 20 c_2 \rho k Re)$$

Effect of Production Limiter for the Chien $k-\epsilon$ Model

RAE Airfoil Analysis, Turbulent Viscosity Contours

Mach = 0.725, $\alpha = 2.55$ deg., $Re = 6.5$ Million

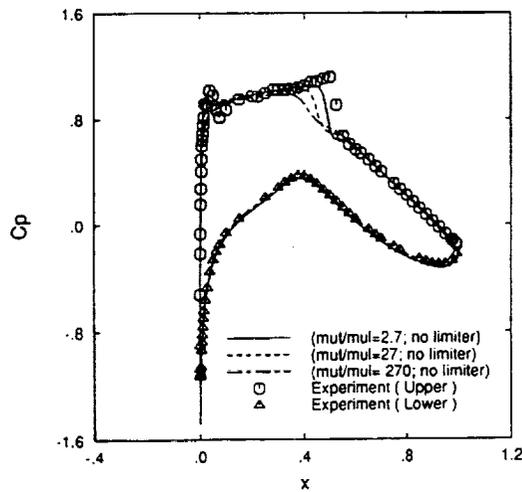


RAE Airfoil Analysis

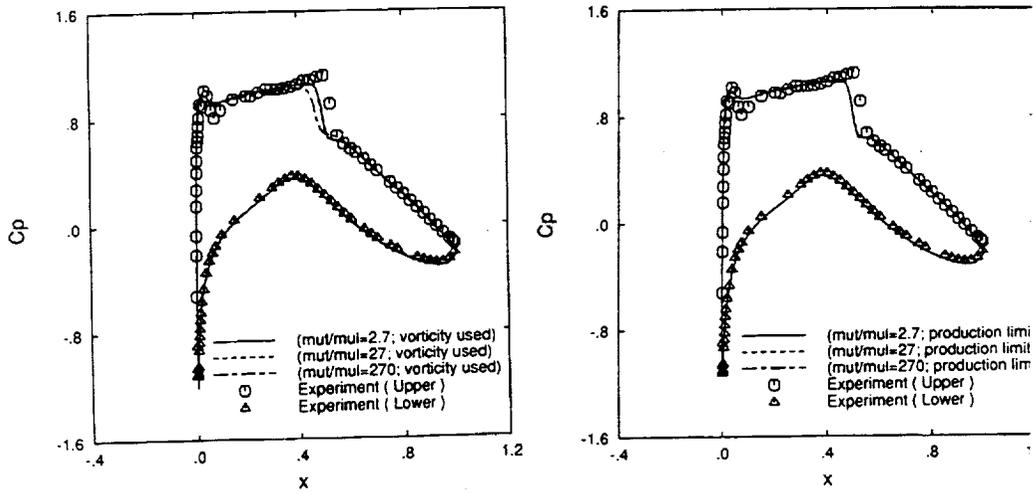
$M_\infty = 0.725$, $\alpha = 2.55^\circ$, $Re = 6.5$ Million

Effect of Freestream Turbulence Level on Surface Pressure

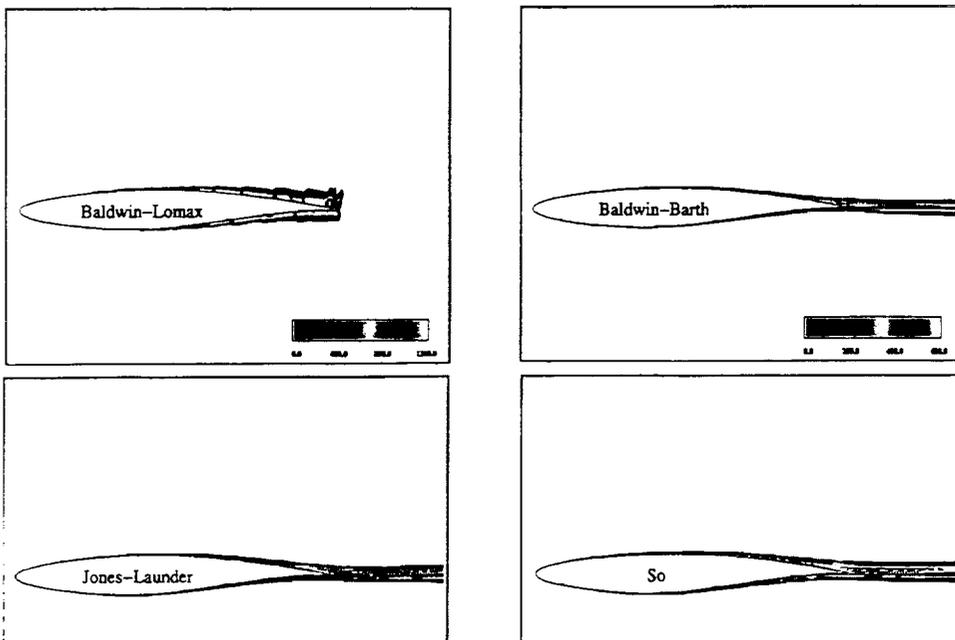
Chien $k - \epsilon$ Turbulence Model



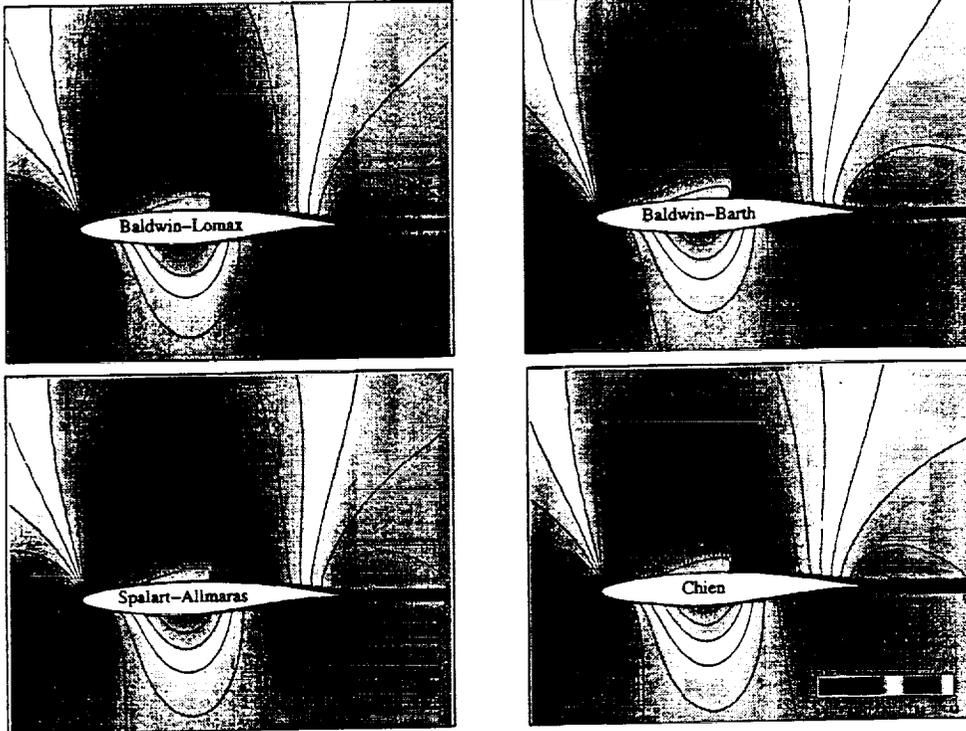
RAE Airfoil Analysis
 $M_\infty = 0.725$, $\alpha = 2.55^\circ$, $Re = 6.5$ Million
Production Limiter Used
Chien $k - \epsilon$ Turbulence Model



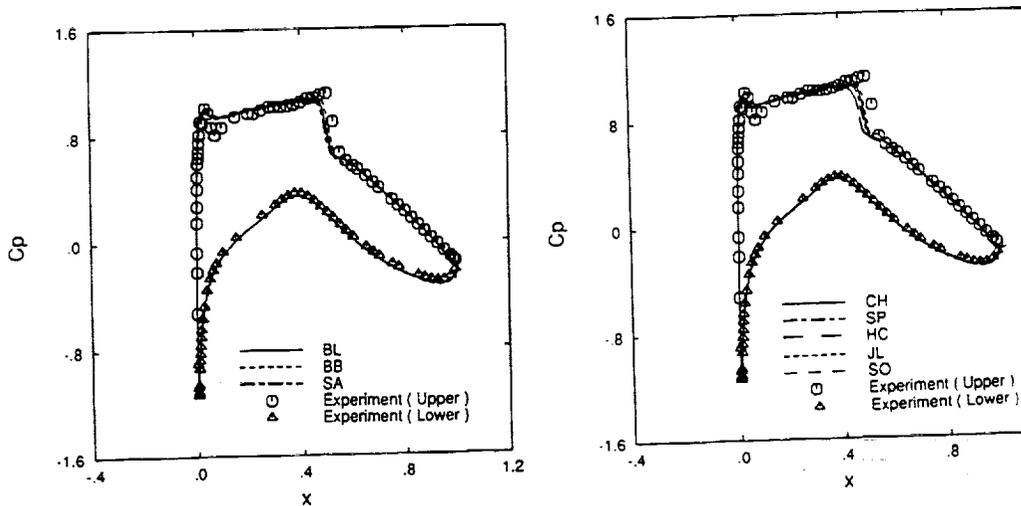
RAE Airfoil Analysis, Turbulent Viscosity Contours
Mach = 0.725, $\alpha = 2.55$ deg., $Re = 6.5$ Million



RAE Airfoil Analysis, Mach Contours
 Mach = 0.725, $\alpha = 2.55$ deg., Re = 6.5 Million

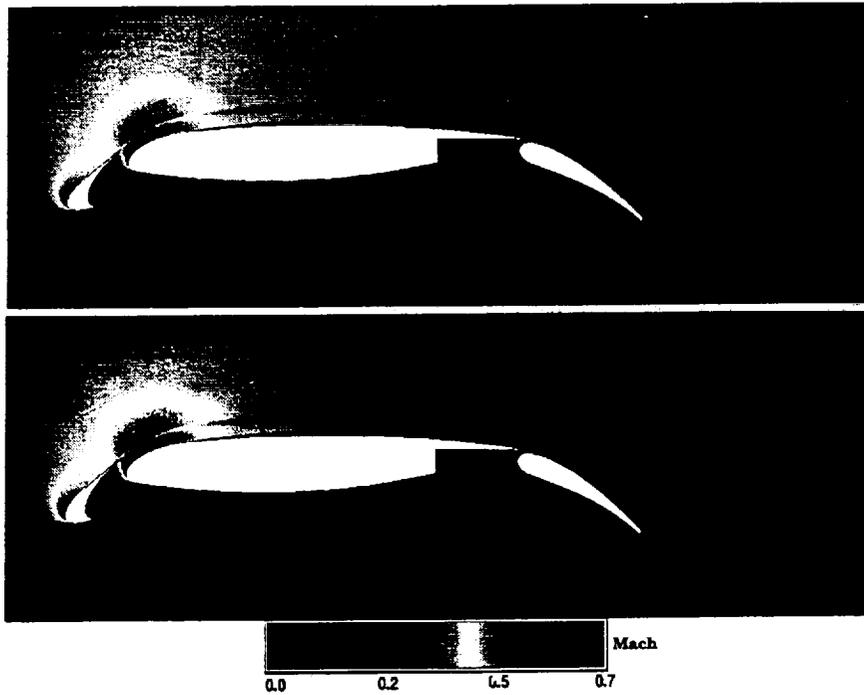


RAE Airfoil Analysis
 $M_\infty = 0.725$, $\alpha = 2.55^\circ$, Re = 6.5 Million
 Effect of Turbulence Model on Surface Pressure



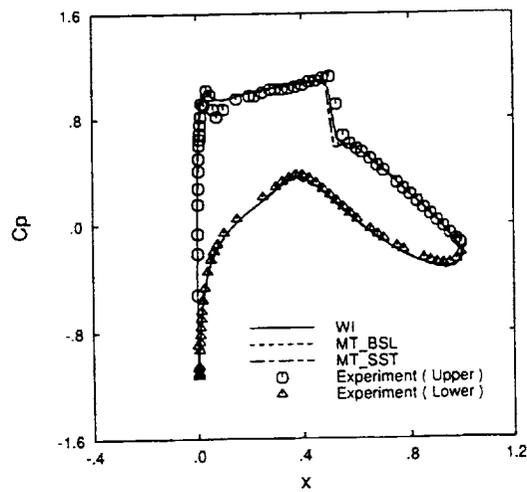
NASTD Solution of MDA Three-Element High-Lift System

M = 0.2, AOA = 16.21



RAE Airfoil Analysis

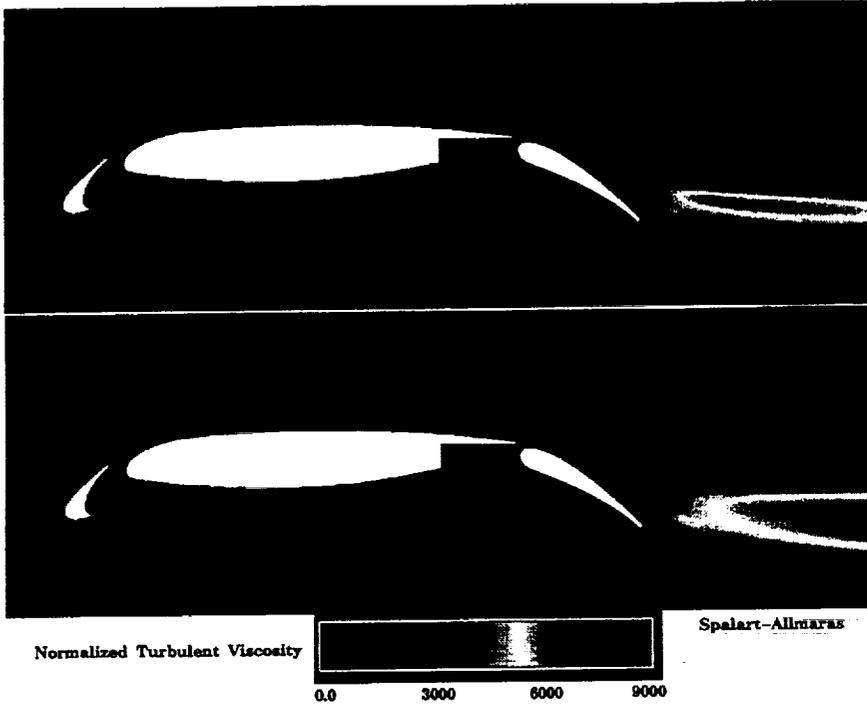
$M_\infty = 0.725$, $\alpha = 2.55^\circ$, $Re = 6.5$ Million
Effect of Turbulence Model on Surface Pressure



NASTD Solution of MDA Three-Element High-Lift System

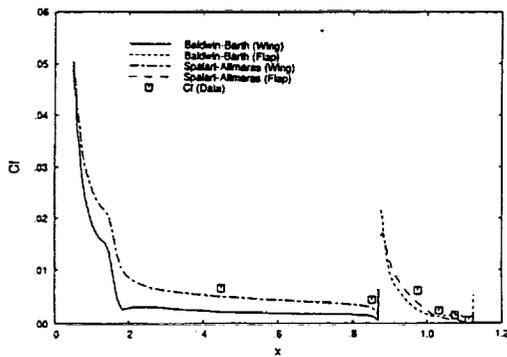
M = 0.2, AOA = 16.21

Baldwin-Barth

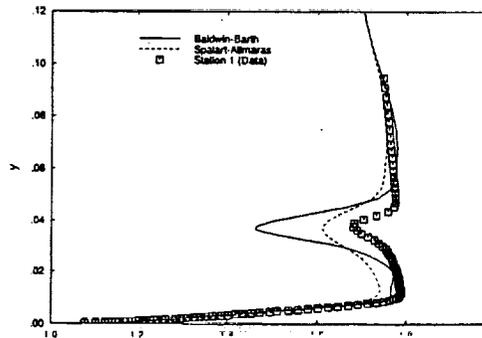


More Accurate Solutions Have Been Obtained With One-Equation Spalart-Allmaras Turbulence Model

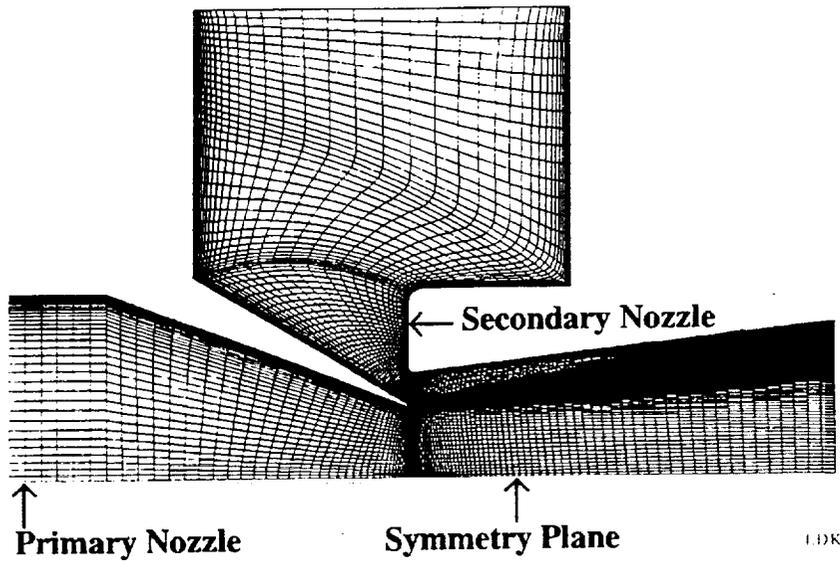
Skin Friction Coefficients on the upper Surfaces



Velocity Profile at Station 1 on the Wing (M=0.2, $\alpha=16.21$)



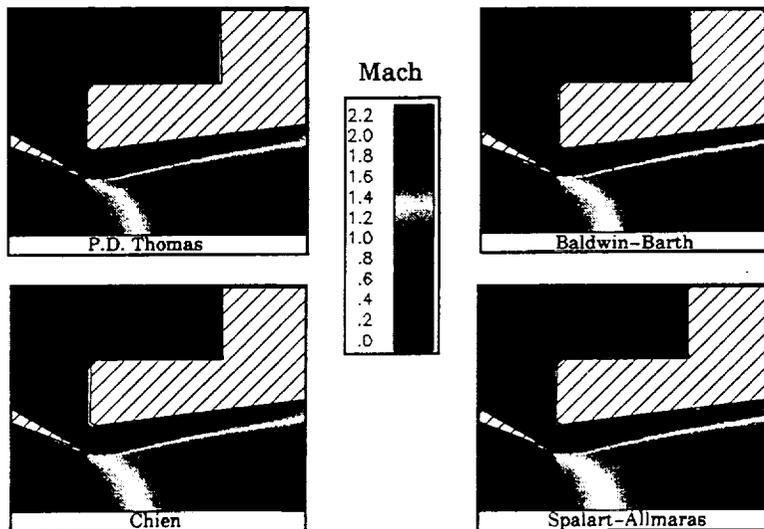
Four-Zone Grid for an Ejector Nozzle



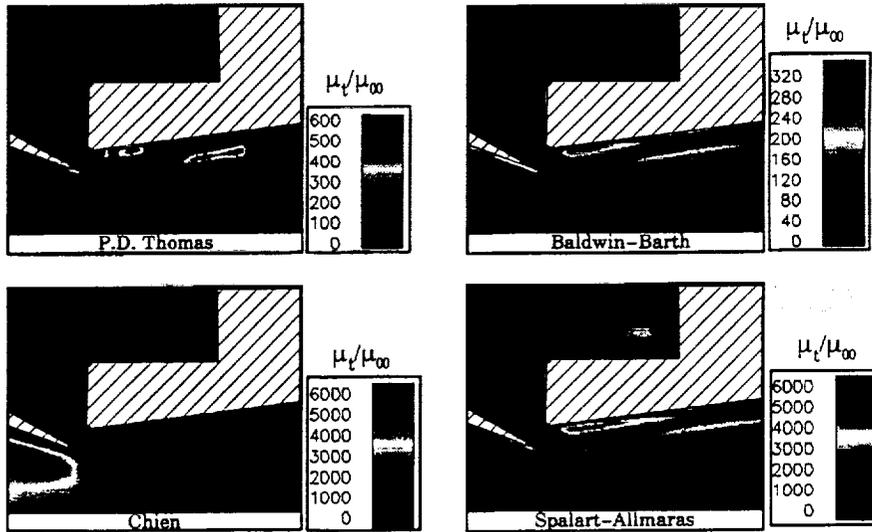
Single Slot Ejector Analysis

NPR=14., Pts/Ptp=.34

Mach Number Contours from Several Turbulence Models



Single Slot Ejector Analysis
 NPR=14., $P_{ts}/P_{tp}=0.34$
Eddy Viscosity from Several Turbulence Models



Single-Slot Ejector Nozzle Analysis

$NPR = 14, P_{ts}/P_{tp} = 0.34$

$\mu_t/\mu_l \approx 100$

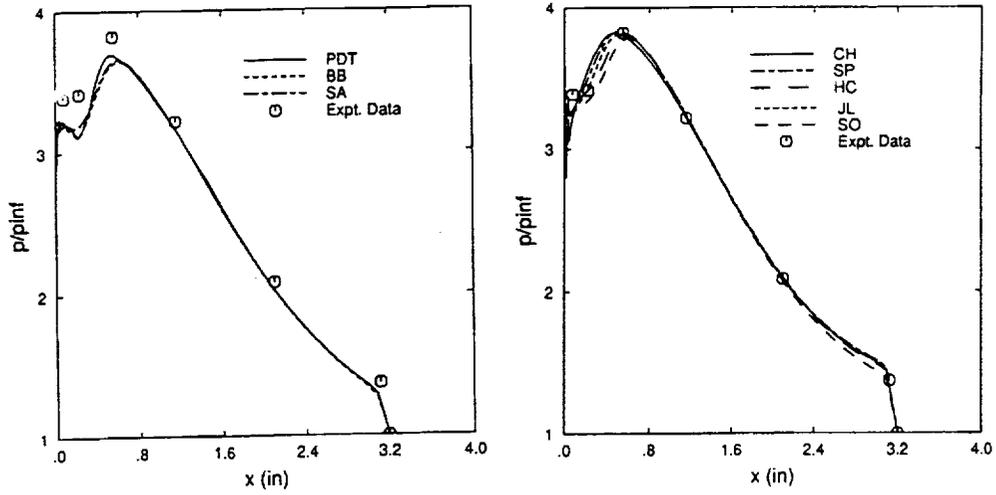
Comparison of Predicted Ejector Flow Rates

Model	W_s/W_p	% Error
Experiment	0.1010	—
Thomas/Baldwin-Lomax	0.1108	+9.7
Baldwin-Barth	0.1129	+11.8
Spalart-Allmaras	0.1146	+13.5
Chien $k - \epsilon$	0.1168	+15.6
Jones-Launder $k - \epsilon$	0.1126	+11.5
Speziale $k - \epsilon$	0.1127	+11.6
So $k - \epsilon$	0.1148	+13.7
Huang-Coakley $k - \epsilon$	0.1112	+10.1

Single Slot Ejector Nozzle

Surface Static Pressure Comparison with Experimental Data

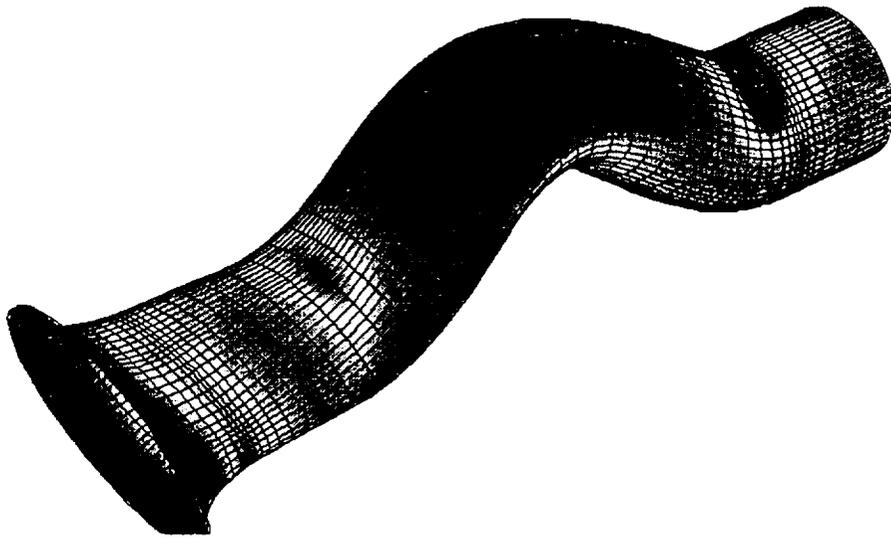
$$NPR = 14.0, P_{t_s}/P_{t_p} = 0.34$$



Offset Diffuser Analysis

$A_e/A_t=1.6$, $L/D=4.5$, Design Pressure Ratio

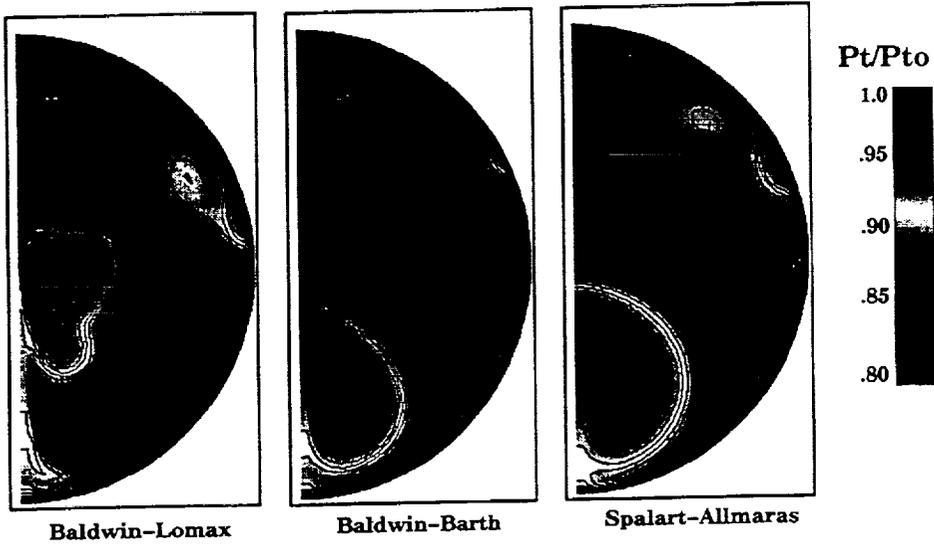
Surface Pressure and Computational Mesh



Offset Diffuser Analysis

$A_e/A_t=1.6$, $L/D=4.5$, Design Pressure Ratio

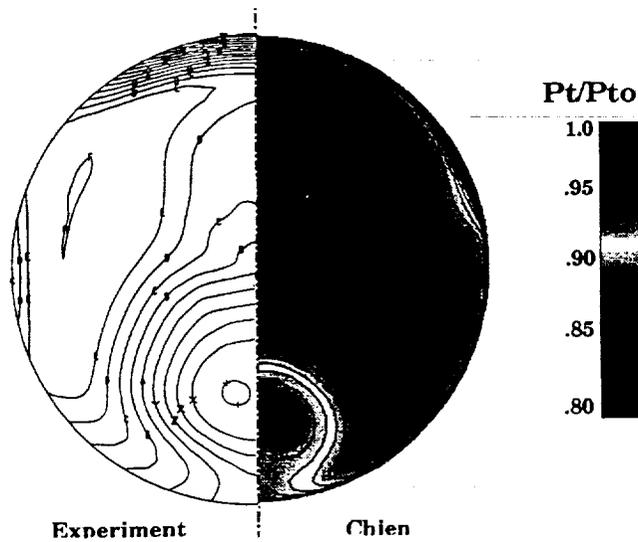
Comparison of Engine Face Total Pressures



Offset Diffuser Analysis

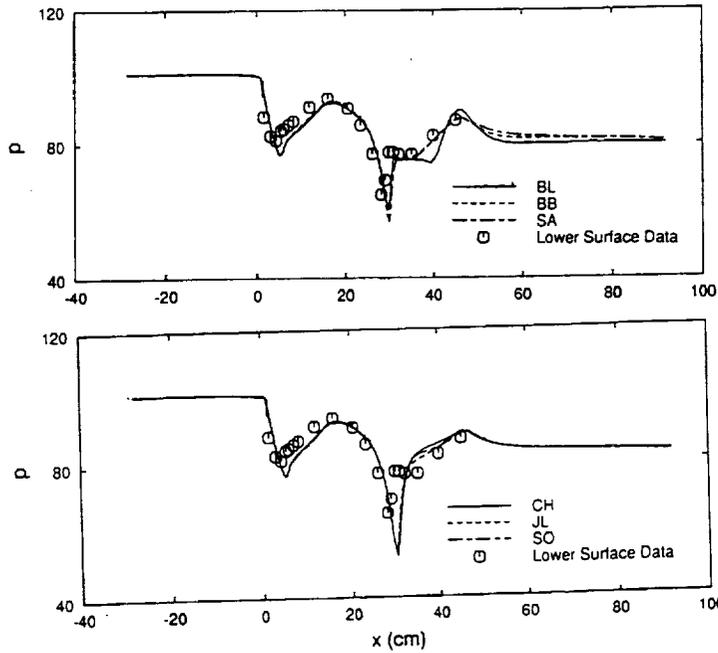
$A_e/A_t=1.6$, $L/D=4.5$, Design Pressure Ratio

Comparison of Engine Face Total Pressures



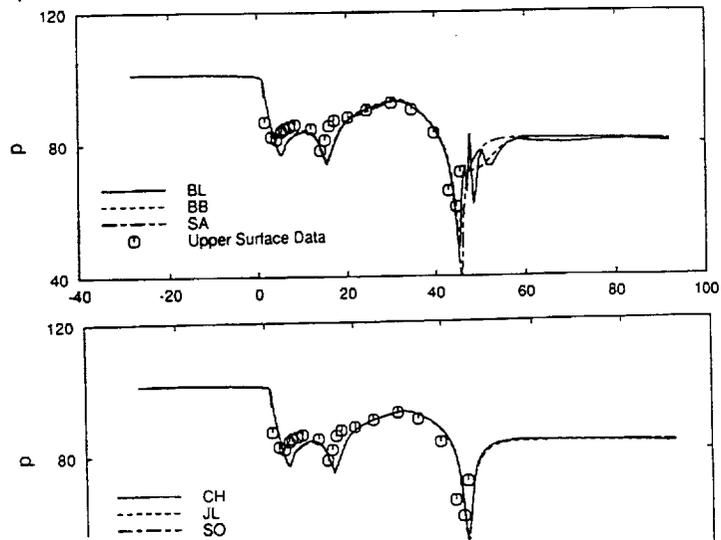
Offset Diffuser Analysis

Lower Centerline Surface Static Pressure
 $A_e/A_t = 1.6$, $L/D = 4.5$, Design Pressure Ratio



Offset Diffuser Analysis

Upper Centerline Surface Static Pressure
 $A_e/A_t = 1.6$, $L/D = 4.5$, Design Pressure Ratio



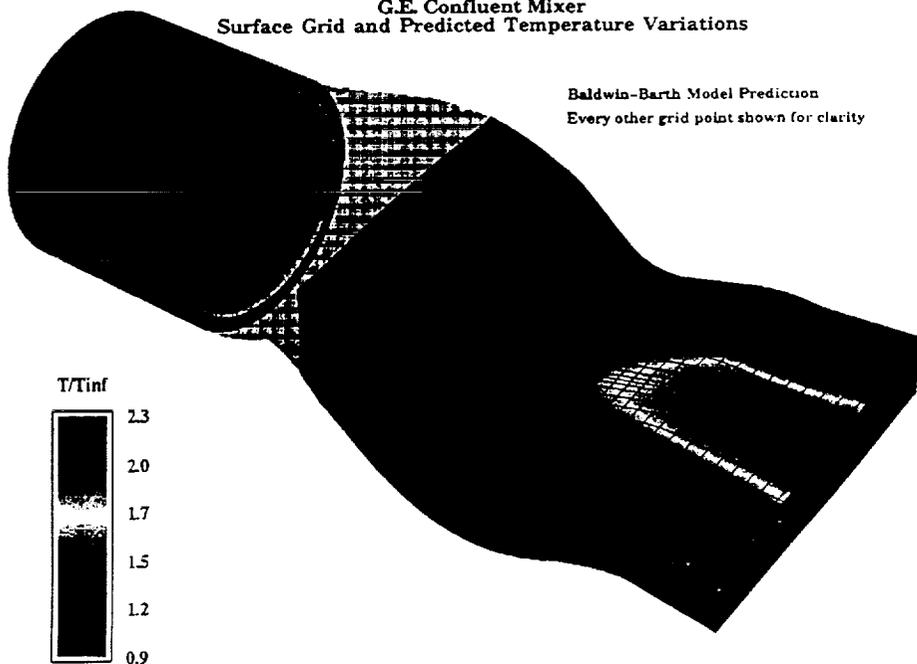
Three-Dimensional Highly Offset Diffuser

$A_e/A_t = 1.6$, $L/D = 4.5$, Design Pressure Ratio

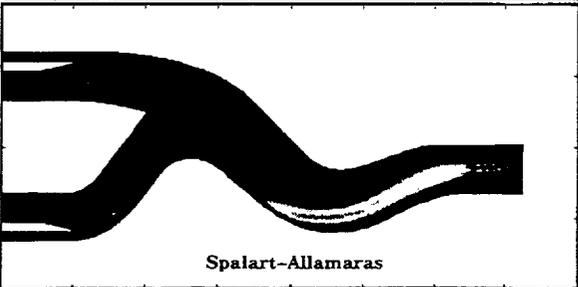
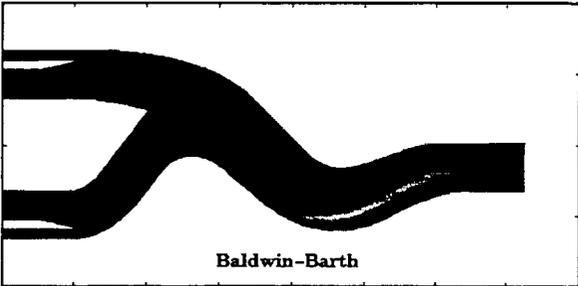
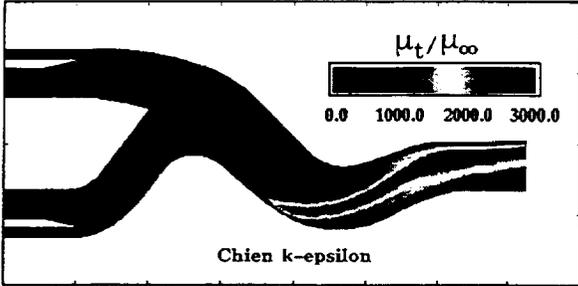
Comparison of Engine Face Parameters

Model	$P_{t_{avg}}/P_{t_{\infty}}$	$P_{t_{min}}/P_{t_{\infty}}$	$\frac{P_{t_{max}} - P_{t_{min}}}{P_{t_{avg}}}$
Experiment	0.958	0.890	0.114
Baldwin-Lomax	0.936	0.708	0.292
Baldwin-Barth	0.944	0.735	0.265
Spalart-Allmaras	0.955	0.860	0.140
Chien $k - \epsilon$	0.970	0.894	0.106
Jones-Launder $k - \epsilon$	0.966	0.896	0.104
So $k - \epsilon$	0.975	0.888	0.112

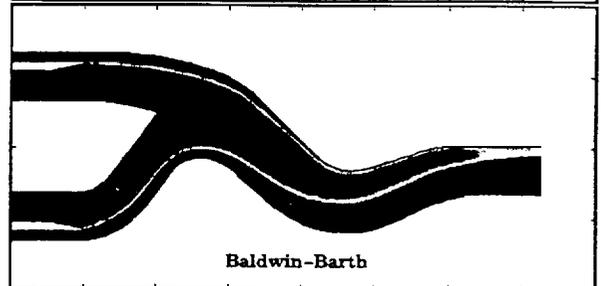
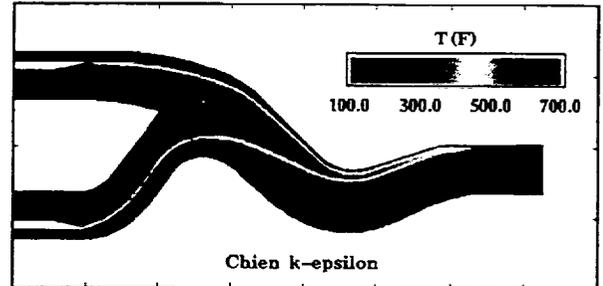
G.E. Confluent Mixer
Surface Grid and Predicted Temperature Variations



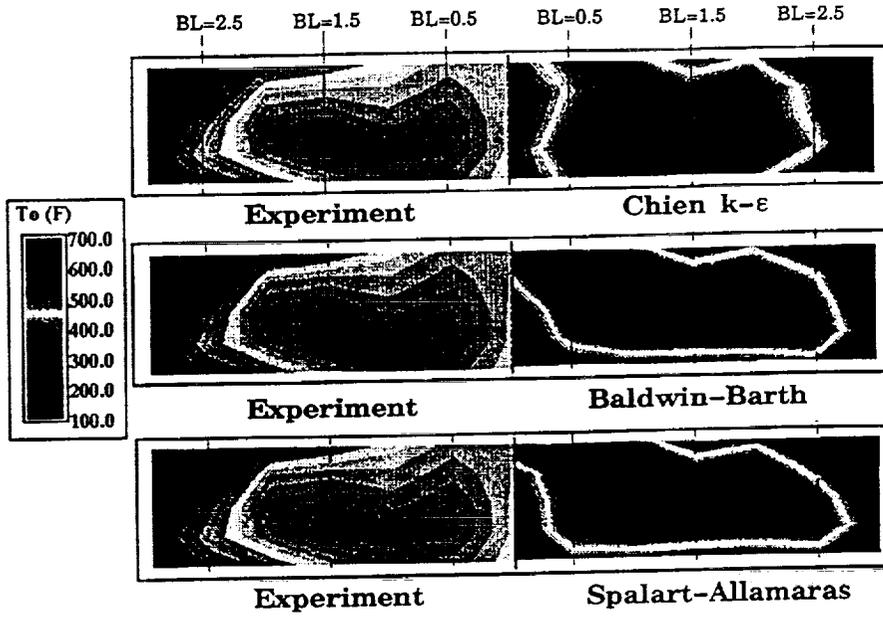
Centerline Eddy Viscosity Contours



Centerline Temperature Contours



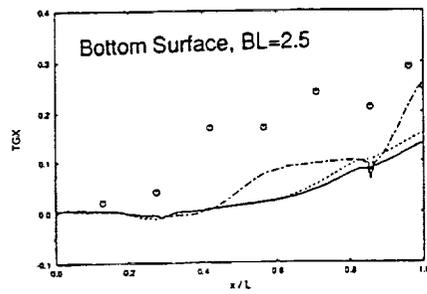
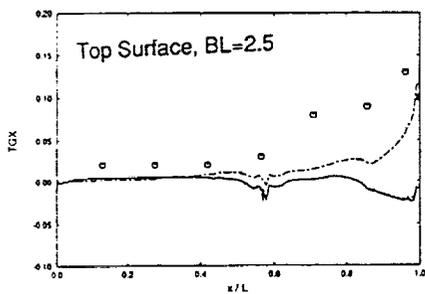
Comparison of Throat Total Temperatures



GE Slot Cooled Nozzle, Confluent Mixer

Surface Temperature Distributions,

$$TGX = (T_I - T_{I_{cold}}) / (T_{I_{hot}} - T_{I_{cold}})$$

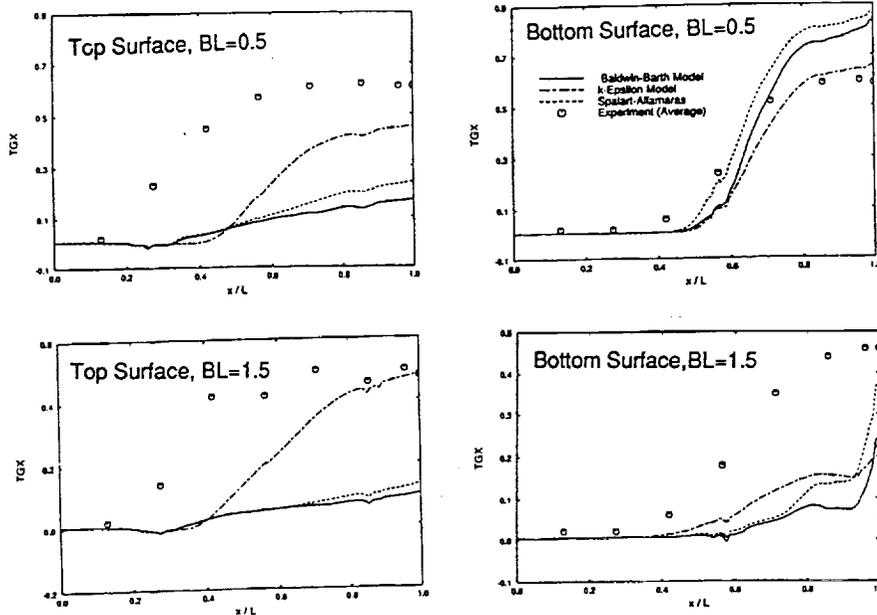


- Baldwin-Barth Model
- - - k-Epsilon Model
- · · Spalart-Allamaras
- Experiment (Average)

GE Slot Cooled Nozzle, Confluent Mixer

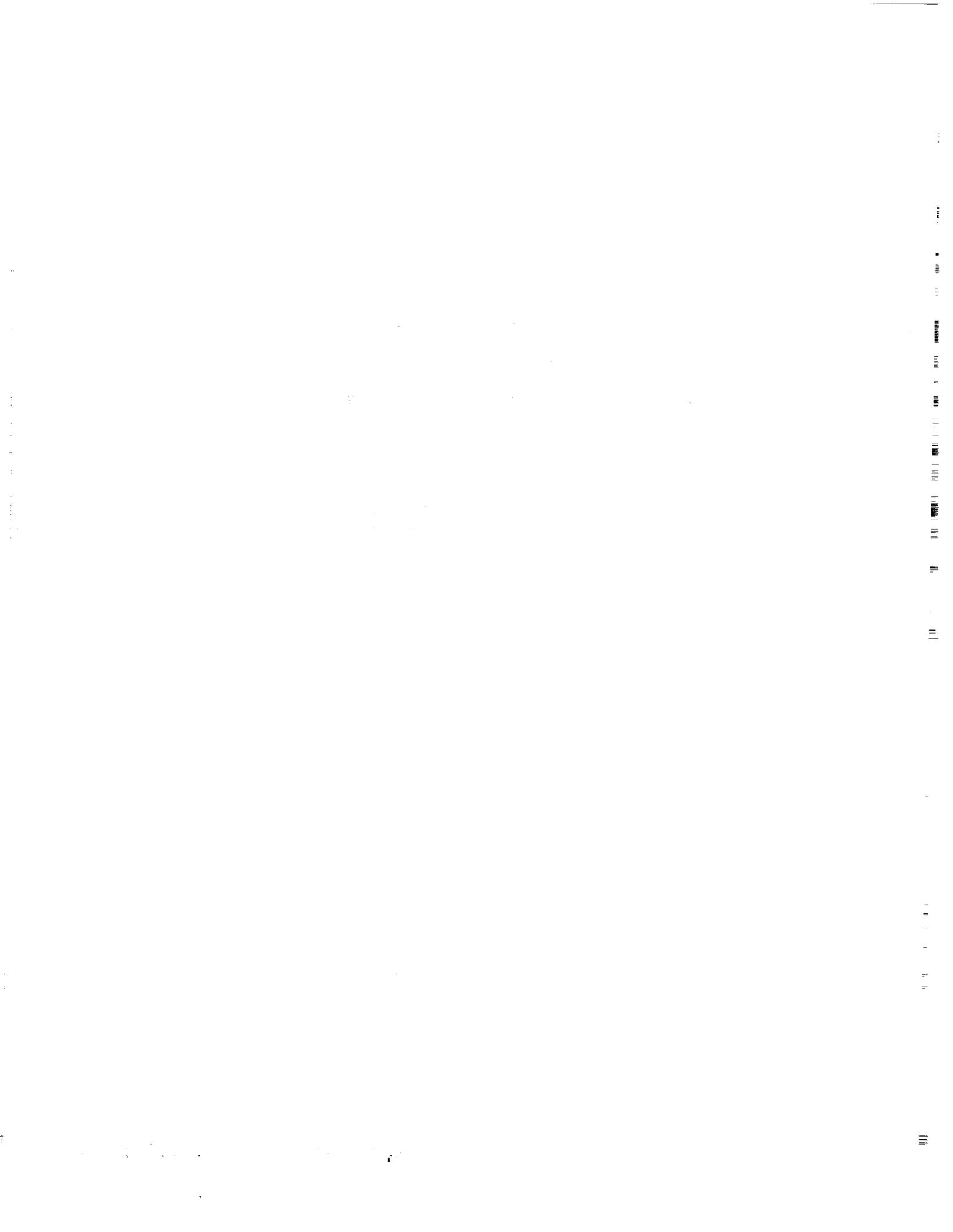
Surface Temperature Distributions,

$$TGX = (T_I - T_{I,cold}) / (T_{I,hot} - T_{I,cold})$$



Summary of Turbulence Modeling at McDonnell Douglas Aerospace

- The one-equation models have replaced the algebraic models as the baseline turbulence models.
- The Spalart-Allmaras one-equation model consistently performs better than the Baldwin-Barth model, particularly in the log-layer and free shear layers. Also, the Spalart-Allmaras model is not grid dependent like the Baldwin-Barth model.
- No general turbulence model exists for all engineering applications.
- The Spalart-Allmaras one-equation model and the Chien $k - \epsilon$ models are the preferred turbulence models.
- Although the two-equation models often better predict the flowfield, they may take from two to five times the CPU time.
- Future directions are in further benchmarking the Menter blended $k - \omega / k - \epsilon$ and algorithmic improvements to reduce CPU time of two-equation model.



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OUTLINE

- Geometry and flow configuration
- Effect of y^+ on heat transfer computations
- Standard and Extended $k-\epsilon$ turbulence model results with wall function
- Low-Re model results (the Lam-Bremhorst model without wall function)
- A criterion for flow reversal in a radially rotating square duct
- Summary

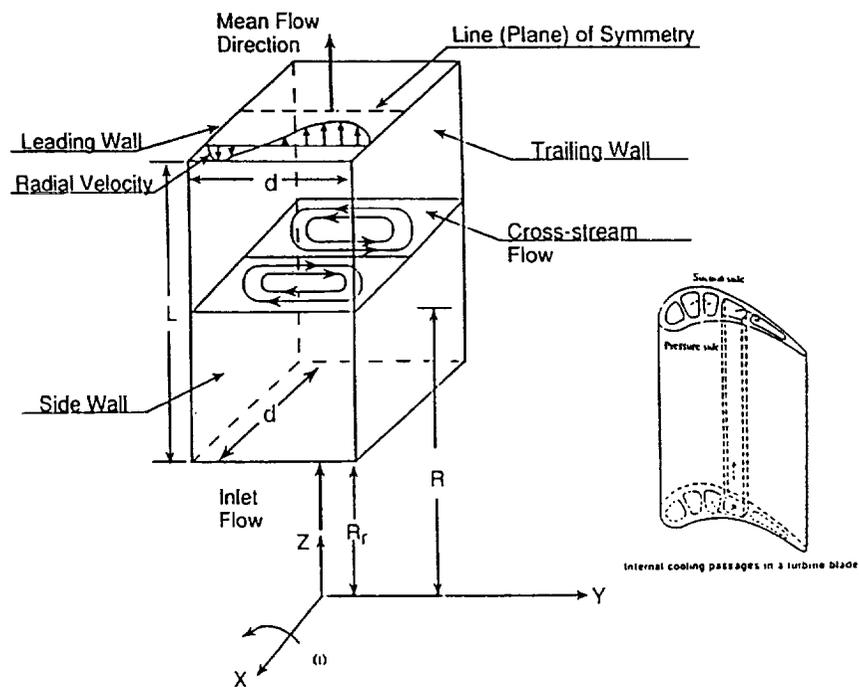


Fig. 1-Illustration of geometry and physics of flow

TWO-EQUATION TURBULENCE MODELS

$$\mu_t = f_{\mu} C_{\mu} \rho k^2/\epsilon$$

$$\frac{D(\rho k)}{Dt} = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{Pr_k} \frac{\partial k}{\partial x_i} \right) + \rho(G_k - \epsilon)$$

$$\frac{D(\rho \epsilon)}{Dt} = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{Pr_{\epsilon}} \frac{\partial \epsilon}{\partial x_i} \right) + f_1 C_1 \frac{\epsilon}{k} \rho G_k - f_2 C_2 \rho \frac{\epsilon^2}{k} + C_3 \rho \frac{G_k^2}{k}$$

where $G_k = \frac{\mu_t}{\rho} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j}$; $C_{\mu} = 0.09$

Standard k-ε model:

$$Pr_k = 1.0, Pr_{\epsilon} = 1.3, C_1 = 1.44, C_2 = 1.92, C_3 = 0.0, f_1 = 1.0, f_2 = 1.0, \text{ and } f_{\mu} = 1.0$$

Extended k-ε model:

$$Pr_k = 0.89, Pr_{\epsilon} = 1.15, C_1 = 1.15, C_2 = 1.9, C_3 = 0.25, f_1 = 1.0, f_2 = 1.0, \text{ and } f_{\mu} = 1.0$$

Lam-Bremhorst low-Re model:

$$Pr_k = 1.0, Pr_{\epsilon} = 1.3, C_1 = 1.44, C_2 = 1.92, C_3 = 0.0, f_1 = (1 + 0.05/f_{\mu})^3, f_2 = 1 - e^{-R_i^2},$$

and $f_{\mu} = (1 - e^{-0.0165 R_k})^2 (1 + 20.5/R_i)$, where $R_k = k^{1/2} y \rho/\mu$ and $R_i = k^2 \rho/\mu \epsilon$

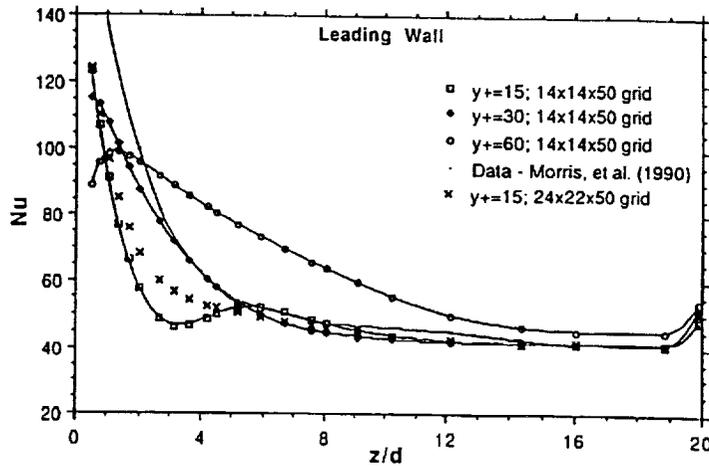


Fig. 2(a)-Effect of y+ and grid size on Nu computation

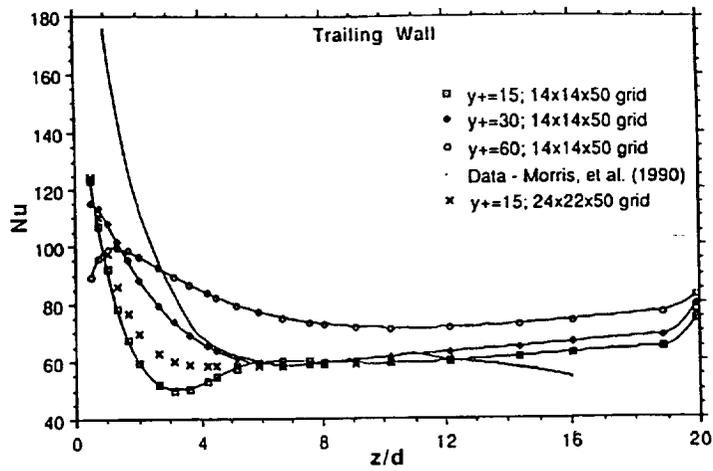


Fig. 2(b)-Effect of y^+ and grid size on Nu computation

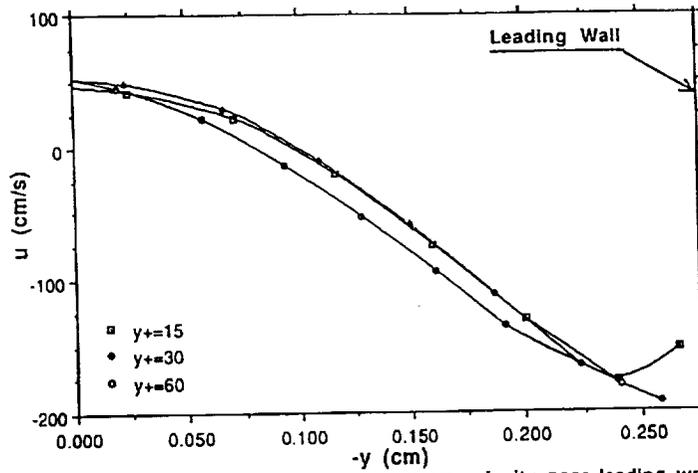


Fig. 2(c)-Effect of y^+ on the cross-stream velocity near leading wall

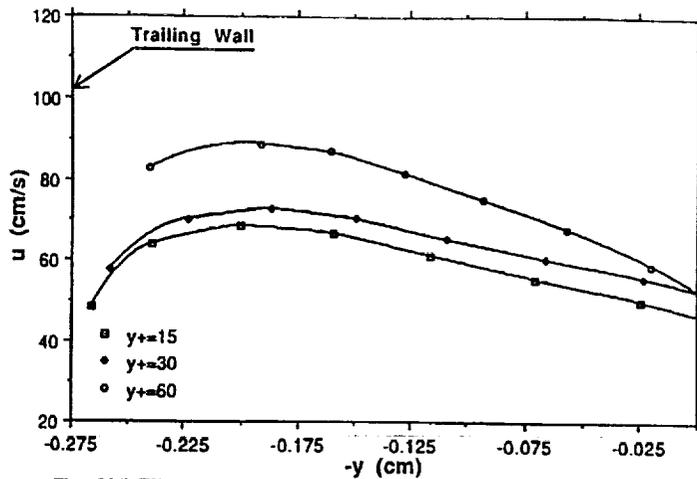


Fig. 2(d)-Effect of y^+ on the cross-stream velocity near trailing wall

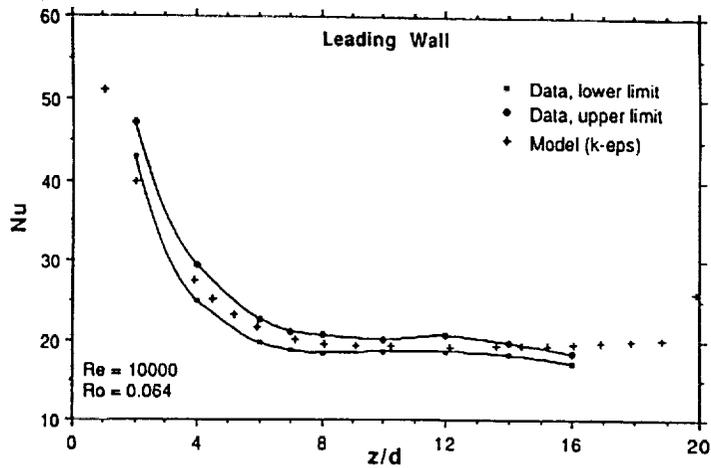


Fig. 3(a)-Comparison of model results with data (Morris & Ghavami-Nasr,1991)

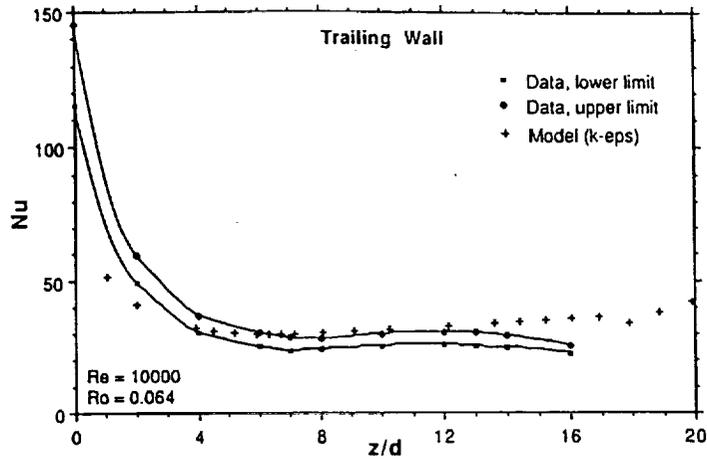


Fig. 3(b)-Comparison of model results with data (Morris & Ghavami-Nasr, 1991)

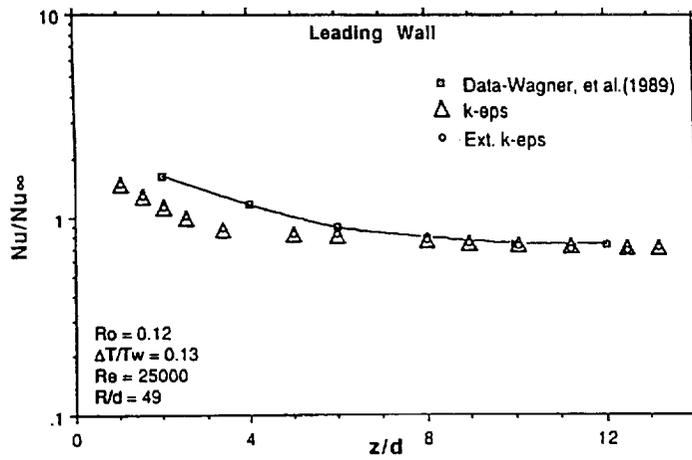


Fig. 4(a)-Comparison of model results with data on leading wall

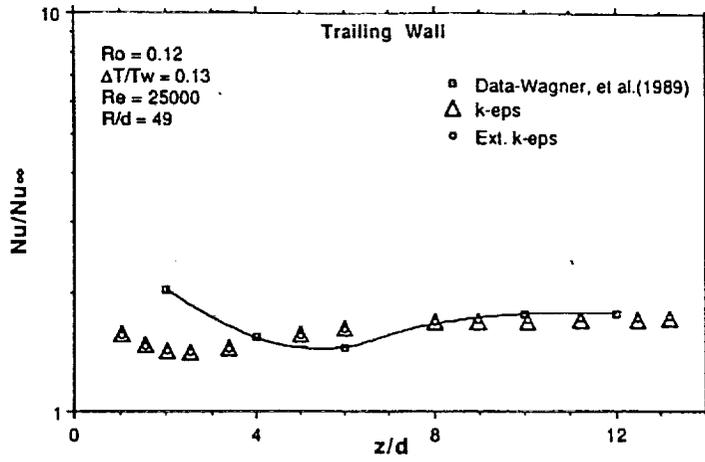


Fig. 4(b)-Comparison of model results with data on trailing wall

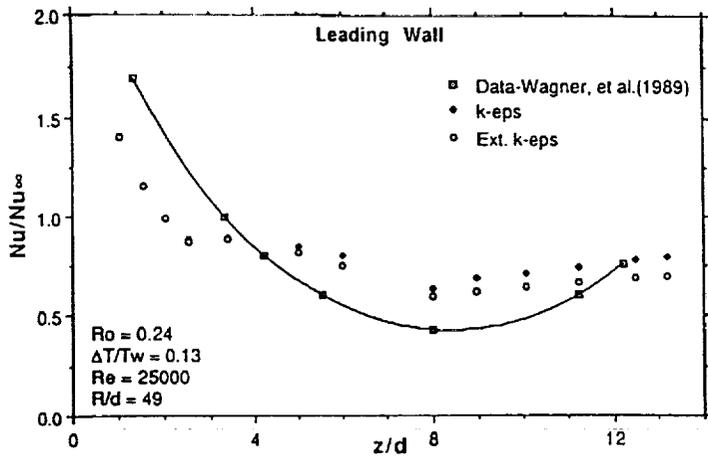


Fig. 4(c)-Comparison of model results with data on leading wall

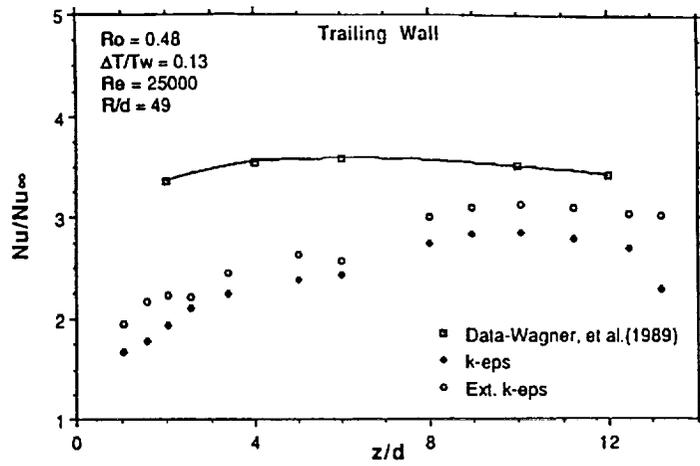


Fig. 4(d)-Comparison of model results with data on trailing wall

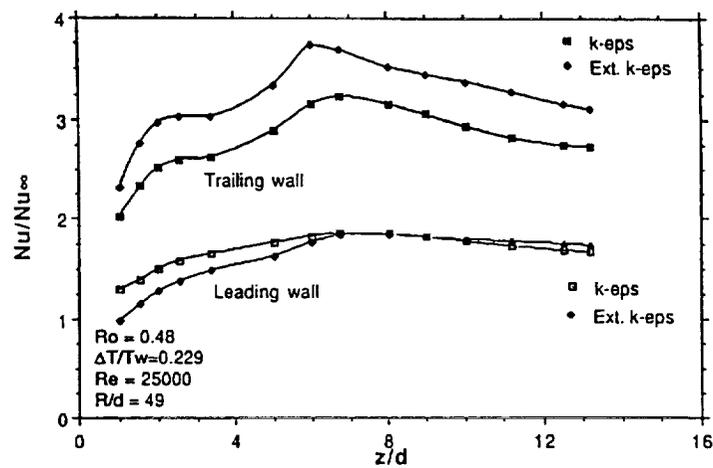


Fig. 5-Comparison of the two model results at high Ro and high density ratio

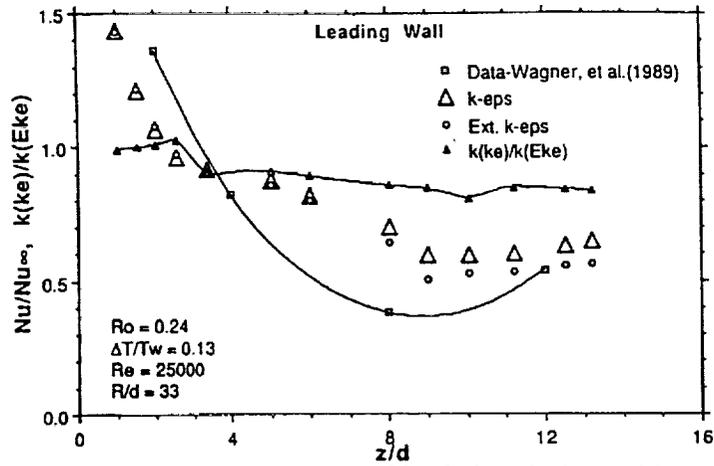


Fig. 6(a)-Plots of Nu-ratio and k-ratio from the two models

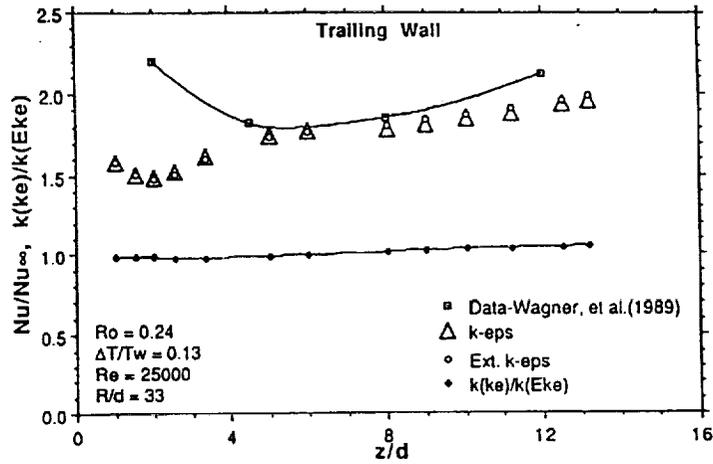


Fig. 6(b)-Plots of Nu-ratio and k-ratio from the two models

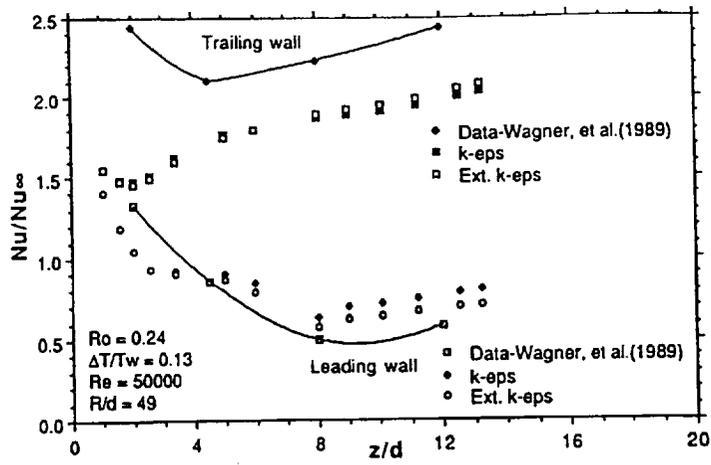


Fig. 7(a)-Comparison on both leading and trailing walls

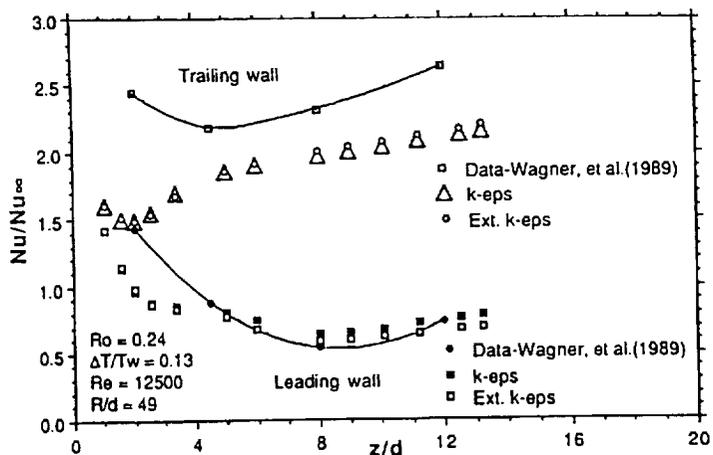


Fig. 7(b)-Comparison on both leading and trailing walls

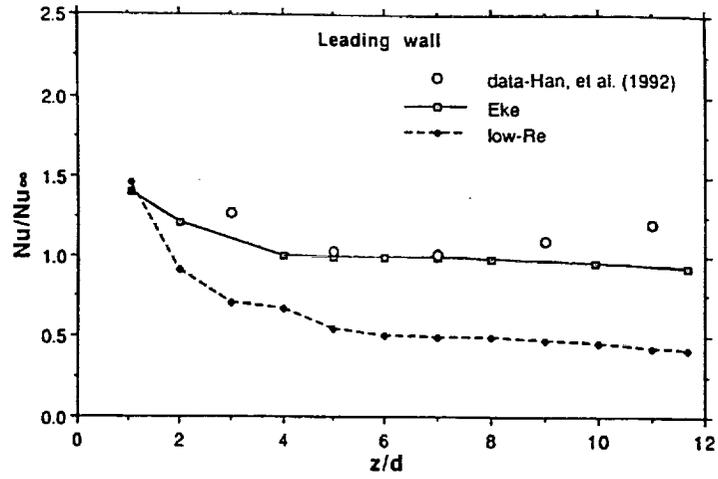


Fig. 8(a)-Comparison of Eke and low-Re results on leading wall (Re=10000, Ro=0.088, Case B)

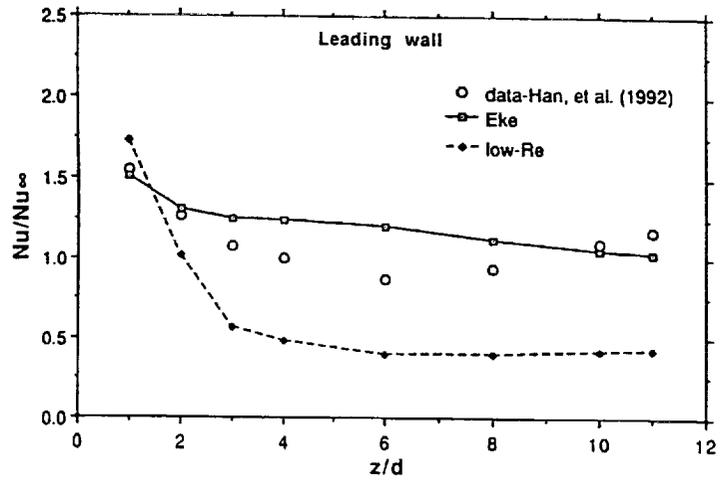


Fig. 8(b)-Comparison of Eke and low-Re results on leading wall (Re=5000, Ro=0.176, Case B)

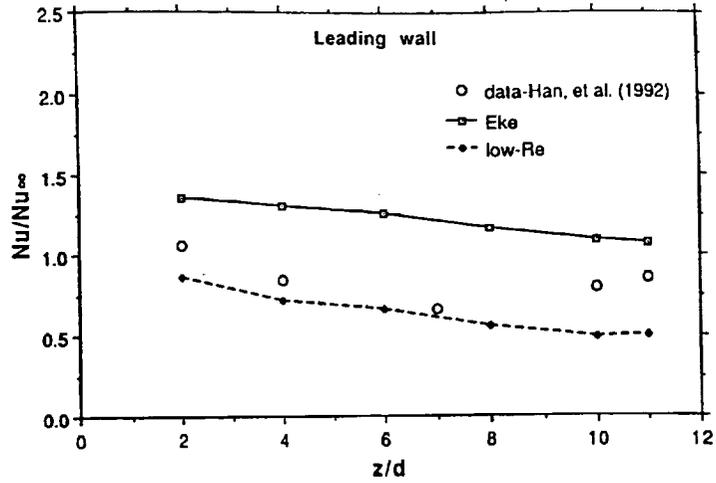


Fig. 8(c)-Comparison of Eke and low-Re results on leading wall (Re=5000, Ro=.176, CaseC)

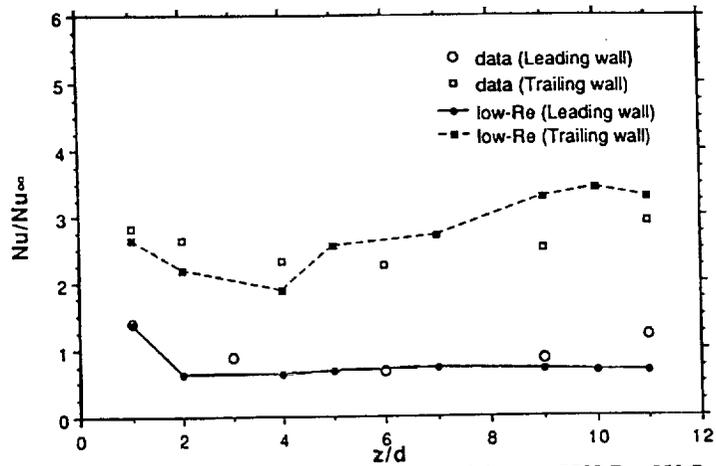


Fig. 8(d)-Comparison of low-Re results with data (Re=2500, Ro=.352, CaseB)

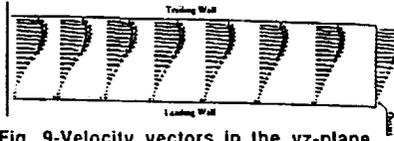


Fig. 9-Velocity vectors in the yz-plane

Table 1 Prediction of Flow Reversal Near the Leading Wall

Ro	$\Delta T/T_w$	R/Δ	Re	Gr/Re ²	Flow Reversal ?	
0.12	0.07	49	25000	0.05	No	
	0.13			0.09	No	
	0.23			0.16	No	
	0.36			0.26	No	
	0.48			0.34	Yes	
	0.07	196	0.20	No		
		300	0.30	Yes		
0.24	0.07	33	25000	0.13	No	
		49		0.20	No	
		196		0.77	Yes	
		300		1.18	Yes	
	0.13	49			0.36	Yes
					0.45	Yes
					0.65	Yes
	0.07			12500	0.20	No
					0.13	Yes
					0.23	Yes
0.34	0.13	49	25000	0.73	Yes	
				0.16	Yes	
				0.23	Yes	
0.48	0.13	49	25000	1.45	Yes	

SUMMARY

1. Near-wall grid size has a significant effect on the heat transfer calculations when the "wall function" treatment is used. Numerical experiment on the data of Morris et al. (1991) suggests that a y^+ value in the range of 12 to 42 or so yields more accurate results.
2. The extended $k-\epsilon$ turbulence model, while yielding heat transfer results virtually the same as those of standard $k-\epsilon$ model for low rotation-number flows, provides an improvement over the standard $k-\epsilon$ model by up to 15% or so in heat transfer predictions for high rotation number flows.
3. Wall-function $k-\epsilon$ models predict lower (than data) heat transfer at the trailing wall and higher at the leading wall. The need to properly represent the effect of rotation in the $k-\epsilon$ model equations is realized.
4. The low-Reynolds number model utilizes a large number of cells and the convergence rate is very slow in comparison to the high-Reynolds number model using wall function. It is difficult and expensive to obtain a well converged solution with the low-Re turbulence model.

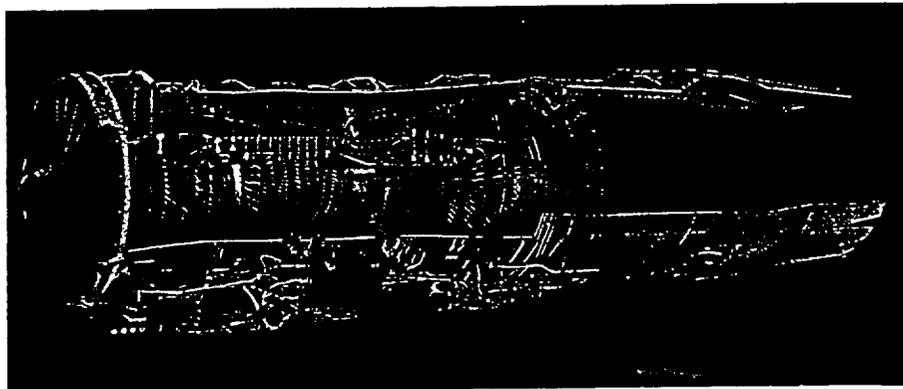
5. The poor agreement of the low-Re model results with the data makes the low-Re model as an unattractive choice for heat transfer computations in rotating radial outward flow at high Rotation number (> 0.24) and high-Reynolds number (25000).
6. The extended version of high-Reynolds number turbulence model in conjunction with wall function yields satisfactory results for flows with isothermal walls as well as uneven wall temperatures. The agreement is within 5-25% of the data with uneven wall temperatures for flows at Reynolds numbers 10000 or higher.
7. For flows at Reynolds number 5000 or lower, the low-Re model predictions are better, especially for the case of uneven wall temperature conditions.
8. The centrifugal buoyancy may cause a flow reversal near the leading wall depending upon the geometry and flow parameters such as rotation number, temperature ratio, mean radius ratio and Reynolds number. For the square-section channel considered here, a criterion of $Bo=Gr/Re^2$ higher than 0.3 is predicted to cause flow reversal near the leading wall for flows at Reynolds number up to 25000.

REFERENCES

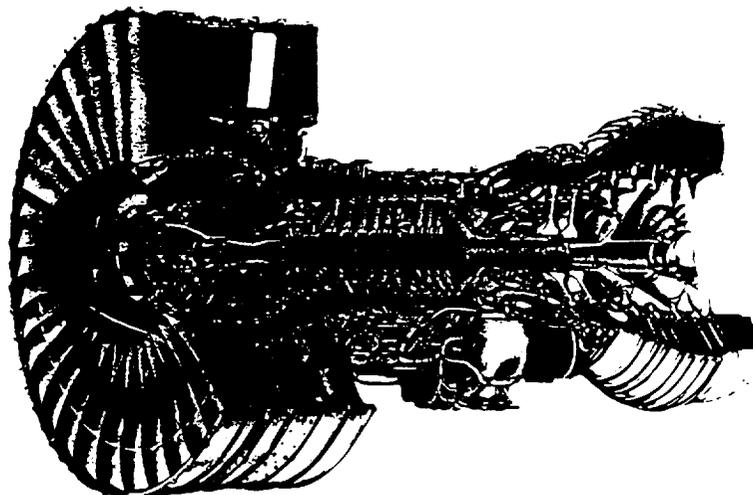
1. Han, J.-C., and Zhang, Y.M., 1992, "Effect of Uneven Wall Temperature on Local Heat Transfer in a Rotating Square Channel With Smooth Walls and Radial Outward Flow," *ASME J. Heat Transfer*, Vol. 114, pp. 850-858.
2. Morris, W.D., and Ghavami-Nasr, G., 1991, "Heat Transfer Measurements in Rectangular Channels with Orthogonal Mode Rotation," *ASME J. Turbomachinery*, Vol. 113, pp. 339-345.
3. Prakash, C., and Zerkle, R., 1991, "Prediction of Turbulent Flow and Heat Transfer in a Radially Rotating Square Duct," *ASME Heat Transfer in Gas Turbine Engines*, HTD-Vol. 188.
4. Tekriwal, P., 1992, "Heat Transfer Predictions with Extended k- ϵ Turbulence Model in Radial Cooling Ducts Rotating in Orthogonal Mode," *ASME HTD - Vol. 226, Fundamentals and Applied Heat Transfer Research for Gas Turbine Engines*, eds. D.E. Metzger and M.E. Crawford, pp. 41-50. Also in *ASME Journal of Heat Transfer*, Vol. 116, 1994, pp. 369-380.
5. Tekriwal, P., 1994, "Prediction of Heat Transfer for Turbulent Flow in Rotating Radial Duct," *Proc. of the 5th Intl. Symp. on Transport Phenomena and Dynamics of Rotating Machinery (ISROMAC 5)*, Vol. A, pp. 673-688.
6. Tekriwal, P., 1994, "Heat Transfer Predictions in Rotating Radial Smooth Channel: Comparative Study of k- ϵ Models with Wall Function and Low-Re Model," Paper No. 94-GT-196, Presented at *The ASME International Gas Turbine and Aeroengine Congress and Exposition*, The Hague, Netherlands, June 1994.
7. Tekriwal, P., 1994, "Centrifugal Buoyancy Driven Reverse Flow Near The Leading Wall of a Rotating Cooling Passage," To be presented at *The ASME Winter Annual Meeting*, Chicago, Illinois, November 1994.
8. Wagner, J.H., Johnson, B.V., and Hajek, T.J., 1989, "Heat Transfer in Rotating Passages with Smooth Walls and Radial Outward Flow," *ASME Gas Turbine and Aeroengine Congress and Exposition*, Paper 89-GT-272.

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F100-PW-200 TURBOFAN ENGINE



PW4000

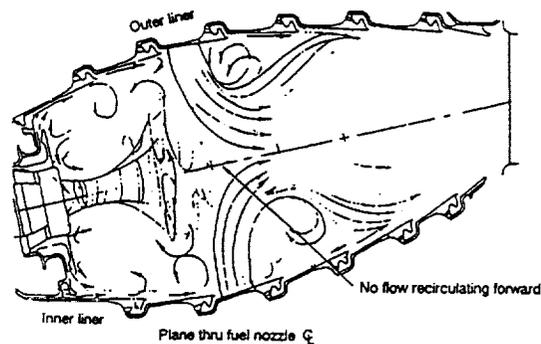


CONTENTS

- Gas Turbine Combustor Flow Physics
- Turbulence Model Investigations
- Turbulent Combustion Modeling
- Present Status and Future Needs

GT COMBUSTOR FLOW PHYSICS

- Key issue is flame stabilization by means of recirculating flow of hot gases and chemically-active species to ensure continuous ignition of fresh reactants.
- Three main mechanisms: 1) axial swirling air jet associated with each fuel introduction; 2) sudden expansion of axial swirling jets; 3) blockage due to radial air jets downstream of fuel sources.

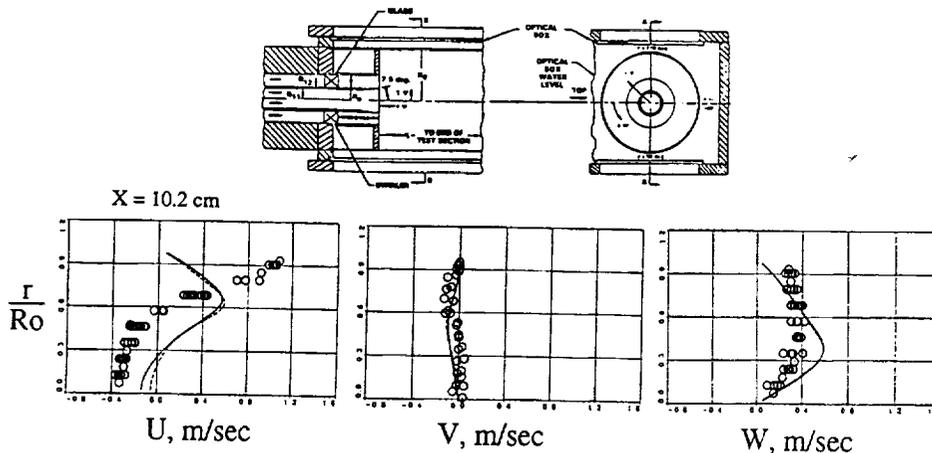


TURBULENCE MODELS SURVEYED

- Following models or modifications have been tested at P&W / UTRC using RANS solvers on building block flows:
 1. low-Re models (complex ducts);
 2. RSTM or SMC (complex ducts, swirling and non-swirling dump combustor);
 3. RNG (pipe, backstep, 180 deg duct);
 4. two-layer near-wall model (internal flows, heat transfer);
 5. realizable algebraic stress model (swirling dump combustor);
 6. compressible turbulence (shear layers, compression corner)
 7. steady vs. unsteady-state solver (bluff-body, compression corner)
- Major difficulty occurs with swirling flows, and failure to predict downstream velocity components.

SWIRLING FLOWS

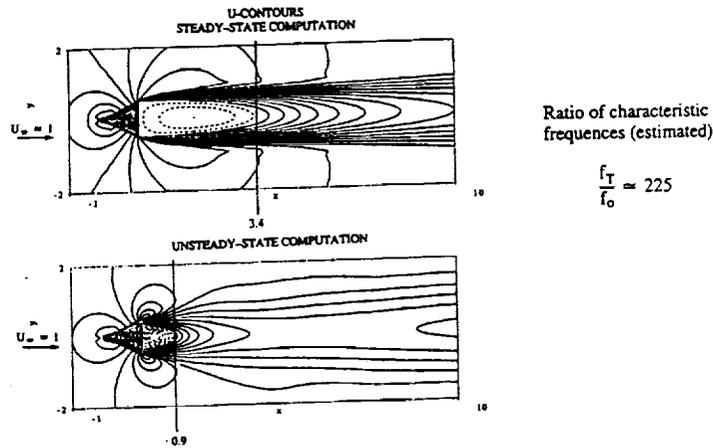
- Benchmark-quality data set provided by Johnson-Roback co-annular combustor with swirl:



- Poor agreement of CFD and data highlights need for improved upstream BC specification (swirler geometry), 3-D, unsteady analysis. Even SMC models fail to reproduce downstream velocity profiles.

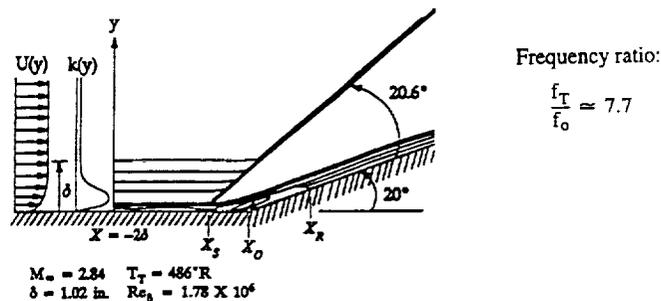
UNSTEADINESS AND FLOW FIELD RESOLUTION

- RANS solvers can predict flow coherence (vortex shedding) when run in an unsteady mode with small Δt .
- Same flow field computed in steady-state sense gives completely unusable results.
- Example: V-gutter flow, computed by Durbin (1994):



UNSTEADINESS AND FLOW FIELD RESOLUTION

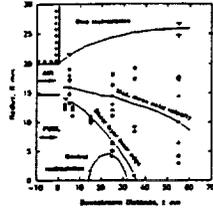
- RANS solvers cannot predict flow oscillations at frequencies near characteristic turbulence frequency.
- Example: Unsteady comp. corner flow of Dolling and Or (1983):



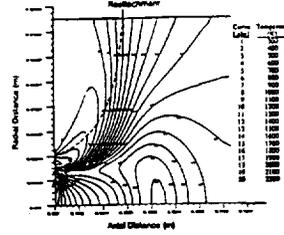
- Separation bubble oscillations (at resonant frequency) not resolved by RANS solver.
- Limitations of steady-state and unsteady-state RANS solvers set by flow characteristic time scales.
True time-accurate solvers (LES, DNS) needed for prediction of all relevant phenomena

TURBULENT COMBUSTION MODELING

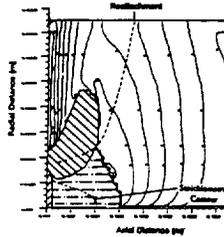
- Eddy Dissipation Concept Model, together with reaction exclusion regions, capable of prediction gross flow features at near LBO conditions (Sturgess et al., 94-GT-433)



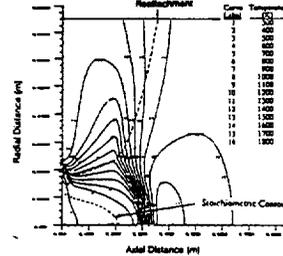
Near-field flow features



EBU-model Temperature field



Reaction exclusion regions



EDC-model Temperature field

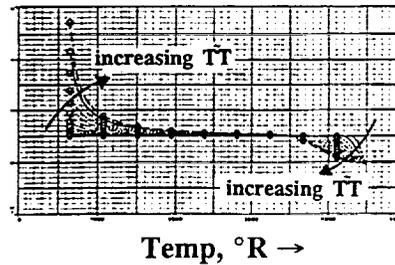
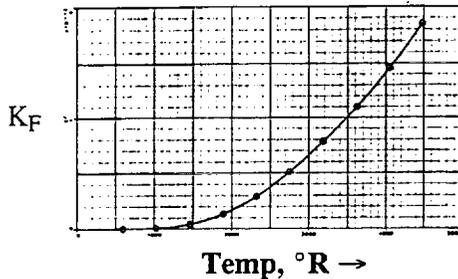
- EDC model, however, fails to predict flame attachment at rich conditions

TURBULENT COMBUSTION MODELING

- Assumed-Pdf method of Girimaji (LaRC Workshop, 1991) used with non-equilibrium kinetics model.

$$\frac{K_{f \text{ turb}}}{K_{f \text{ Lam}}} = \frac{\int_a^b k_f(T) P(T) dT}{k_f(\bar{T})} \quad T_{min} = \max(\bar{T} - \phi \sqrt{T''T''}, T_{low})$$

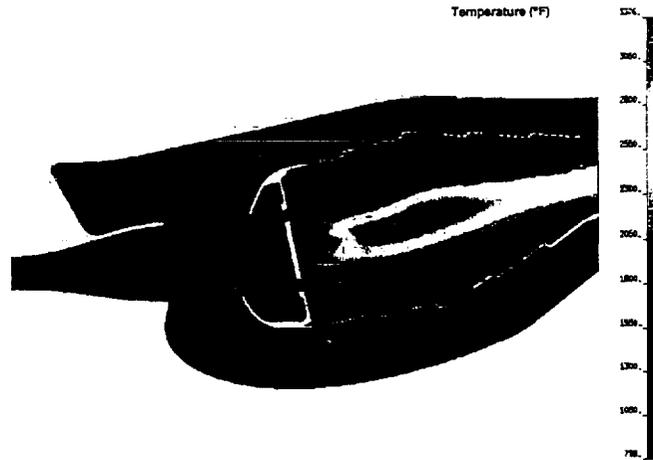
$$T_{max} = \min(\bar{T} + \phi \sqrt{T''T''}, T_{high})$$



- Example: $N + O_2 \rightleftharpoons NO + O$ in extended Zeldovich model
- Results dependent on T_{Low} , T_{High} , ϕ , modeling of $\bar{h}h$ transport equation, etc.
- More testing needed

PRESENT STATUS OF COMBUSTOR MODELING

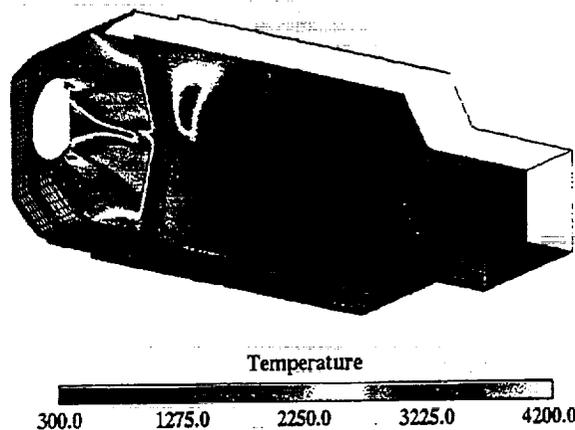
- Corsair (Ryder, P&W) unstructured, unsteady flow solver



- **Example:** Time-dependent combustor flow using engineering boundary conditions, compressor exit to turbine inlet
- Code currently includes standard k- ϵ and EBU combustion model. Additional capabilities being added under "Subsonic Emissions and Combustor Design Code" program with NASA LeRC.

PRESENT STATUS OF COMBUSTOR MODELING

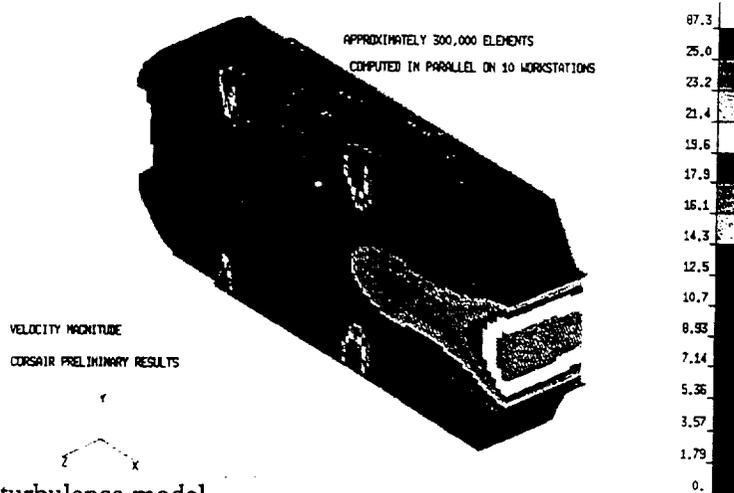
- **Example:** Structured flow solver solution of Task 200 LBO Research Combustor:



- k- ϵ turbulence model
- EBU combustion model for propane fuel
- 285,000 elements

PRESENT STATUS OF COMBUSTOR MODELING

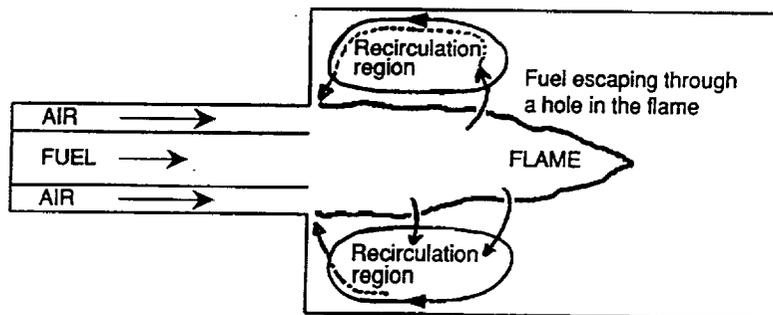
- **Example:** Unstructured flow solver solution of Task 200 LBO Research Combustor:



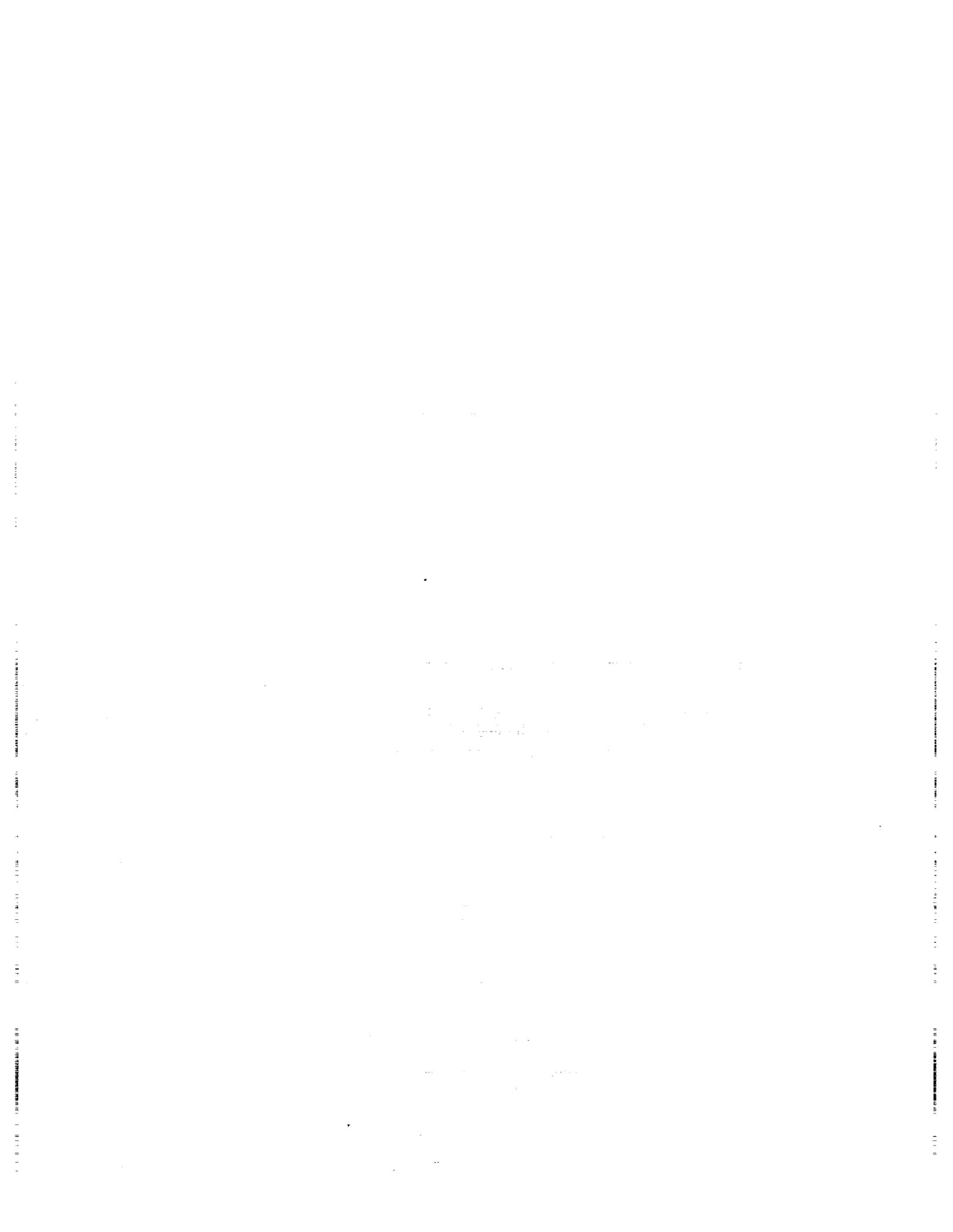
- k- ϵ turbulence model
- EBU combustion model for propane fuel
- Approx. 300,000 elements

TURBULENCE RESEARCH NEEDS

- **Modelling:** Applications / validations of currently available combustion models (β -pdf, Monte Carlo pdf, laminar flamelet) to complex combustor geometry with jet fuel kinetics.
- **Flow Physics:** Accurate numerical description of mechanisms responsible for flame holding, local extinction (LES, DNS); contrast cold flows with heat release flows.



Entrainment of unburned fuel
in the recirculation region



D. Burrus and H. Mongia
GE Aircraft Engines
Cincinnati, Ohio

and

A. Tolpadi, S. Correa, and M. Braaten
GE Corporate Research and Development
Schenectady, New York

**CURRENT COMBUSTION SYSTEM CFD MODELING CAPABILITIES AT GEAE
PROVIDED BY THE *CONCERT CODE***

KEY FEATURES INCLUDE;

FINITE VOLUME, PRESSURE CORRECTION FORMULATION

SECOND ORDER ACCURATE *QUICK* NUMERICS

SINGLE STRUCTURED BODYFITTED GRID

CONVENTIONAL K-E TURBULENCE MODEL WITH LOG WALL FUNCTIONS

AVAILABLE COMBUSTION MODELS INCLUDE;

SINGLE SCALAR PRESUMED SHAPE PDF (FAST CHEMISTRY)

TWO SCALAR PRESUMED SHAPE PDF (REACTION PROGRESS VARIABLE)

TWO STEP EDDY BREAKUP (ARRHENIUS KINETICS)

ZELDOVICH THERMAL NO_x MECHANISM (FORWARD AND REVERSE REACTIONS)

BOTH 2D/AXISYMMETRIC AND FULLY 3D VERSIONS AVAILABLE AND IN DAY TO DAY
USE

CURRENTLY HAVE A USER BASE OF OVER 20 ENGINEERS AT GEAE AND GE-CRD

TYPICALLY APPLIED TO PREDICT COMBUSTOR PERFORMANCE INCLUDING;

EMISSIONS (CO, HC, AND THERMAL NO_x), COMBUSTION EFFICIENCY

EXIT GAS TEMPERATURE RADIAL PROFILE AND PATTERN

GENERAL FLOW FIELD CHARACTERISTICS

CONCERT DEVELOPMENT HISTORY

EFFORT INITIATED IN 1983

INITIAL PRODUCTION VERSION RELEASED TO GEAE USERS IN 1987

FOCUSED TO PROVIDE HIGHLY PRODUCTIVE ENGINEERING ANALYSIS CAPABILITIES

- GRID GENERATION OPTIMIZED FOR THE SPECIFIC GEOMETRY FEATURES OF THE GAS TURBINE COMBUSTOR
 - INCLUDES ROUND DILUTION HOLES, SWIRLER DISCHARGE, AND LINER SLOT FEATURES WITHIN THE GRID
 - EASY INTRODUCTION OF INTERNAL BODIES OF COMPLEX GEOMETRY
- WORKSTATION BASED USER FRIENDLY PRE AND POST PROCESSING FUNCTIONS BUILT AROUND THE SOLVER
- SOLVER HIGHLY OPTIMIZED FOR THE GEAE CRAY C-90 COMPUTER

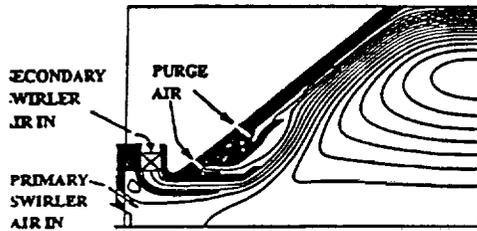
TYPICAL 3D MODEL OF A COMBUSTOR UTILIZING A MESH OF ~100,000 POINTS CAN BE GENERATED, RUN, AND POST PROCESSED WITHIN A SINGLE WORKING DAY!

HAS UNDERGONE CONTINUAL DEVELOPMENT TO IMPROVE AND ENHANCE MODELING CAPABILITIES

- CURRENTLY ON VERSION 3 RELEASE

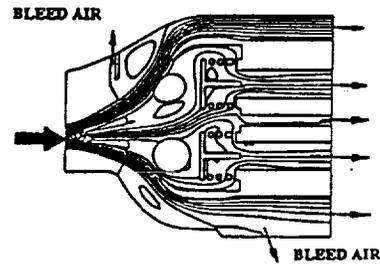
CONCERT CFD MODELING PACKAGE PROVIDES DESIGN ENGINEERS WITH A COST AND TIME EFFECTIVE ANALYSIS TOOL THAT REDUCES DEPENDENCE ON COSTLY COMPONENT RIG TESTING.

COMBUSTION SYSTEM CFD MODELING IN ACTION AT GEAE



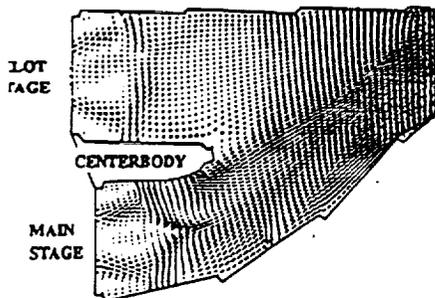
SWIRLCUP/SPRAY MODELING

- RECIRCULATION STRENGTH/SIZE
- FLOW FIELD CHARACTERISTICS
- SPRAY DROPLET TRAJECTORIES
- INPUTS FOR 3D COMBUSTOR MODEL



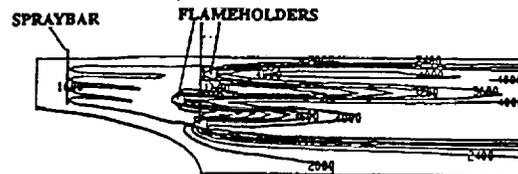
DIFFUSER FLOW MODELING

- P_2 RECOVERIES AND P_1 LOSSES
- FLOW FIELD CHARACTERISTICS



MAIN COMBUSTOR MODELING

- FLOW FIELD CHARACTERISTICS/MIXING
- GAS TEMPERATURES AND PATTERNS
- EMISSIONS/EFFICIENCY



AUGMENTOR MODELING

- FLOW FIELD CHARACTERISTICS/MIXING
- GAS TEMPERATURES AND PATTERNS
- EFFICIENCY

MODELING APPLIED FOR DESIGNING ENGINE COMBUSTION SYSTEMS

PRODUCTION ENGINES	DEMONSTRATOR ENGINES	ADVANCED ENGINES
CFM56-5B DUAL ANNULAR	YF120	A/F-X
GE90	F120	NASA/GE HSCT
CF6-80C LOW EMISSIONS	XTE45 IHPTET PHASE I DEMO	NASA ASI PRELIMINARY CONCEPTS
LM1600 DLE	XTE46 IHPTET PHASE II DEMO	DOE/GE ATS
LM2500 DLE		
LM6000 DLE		

MODELING APPLIED TO IMPROVE FUNDAMENTAL UNDERSTANDING

CFM56-3 AND CFM56-5B NO_x EMISSIONS CHARACTERISTICS DIFFERENCES

CFM56-5A EXIT GAS TEMPERATURE PROFILE SHIFT

F120 PATTERN FACTOR AND RADIAL PROFILE IMPROVEMENT

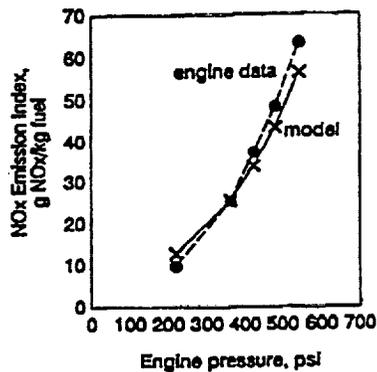
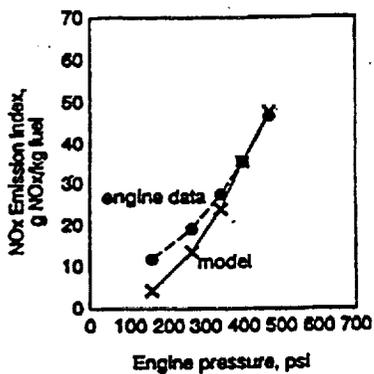
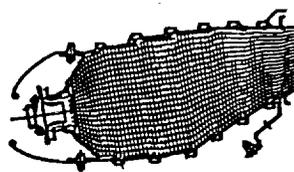
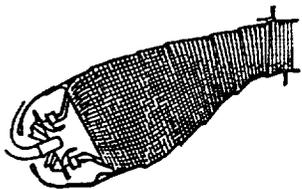
LM2500 CO EMISSIONS REDUCTION EFFORT

CF34 LINER COOLING MOD IMPACT ON CO EMISSIONS

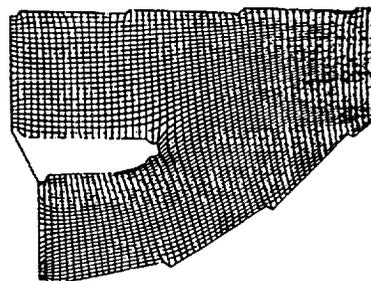
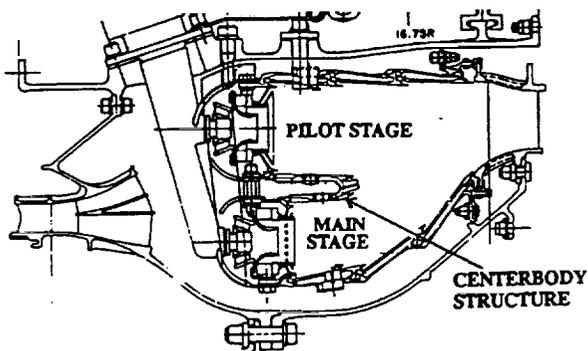
F110X AUGMENTOR MIXER, SPRAYBAR, FLAMEHOLDER INTERACTION OPTIMIZATION

F110-400 AUGMENTOR EXHAUST DUCT LINER FAILURE AND FIX INVESTIGATION

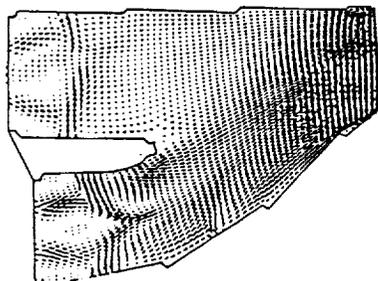
CONCERT3D RESULTS FOR CURRENT PRODUCTION COMBUSTORS



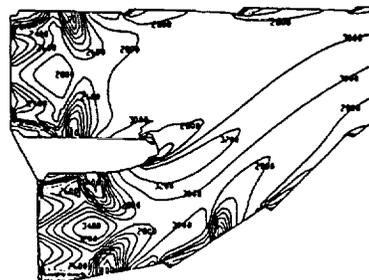
CONCERT3D MODEL OF NASA/GE E3 COMBUSTOR



57X57X25 GRID (81,225 TOTAL MESH POINTS)



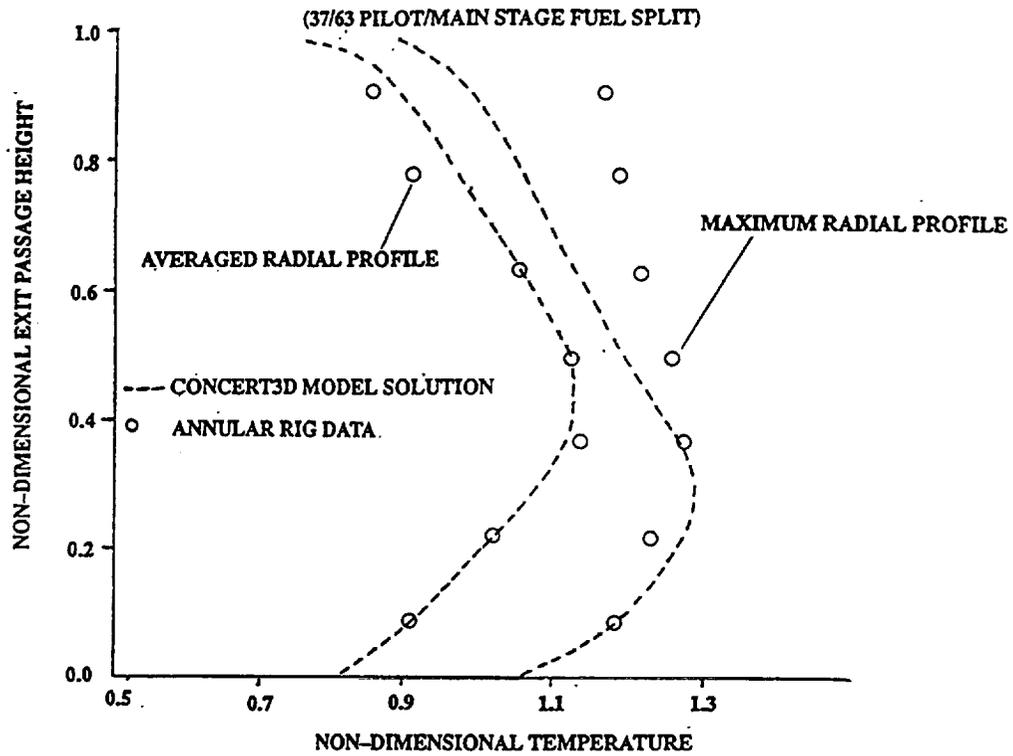
VELOCITY VECTORS



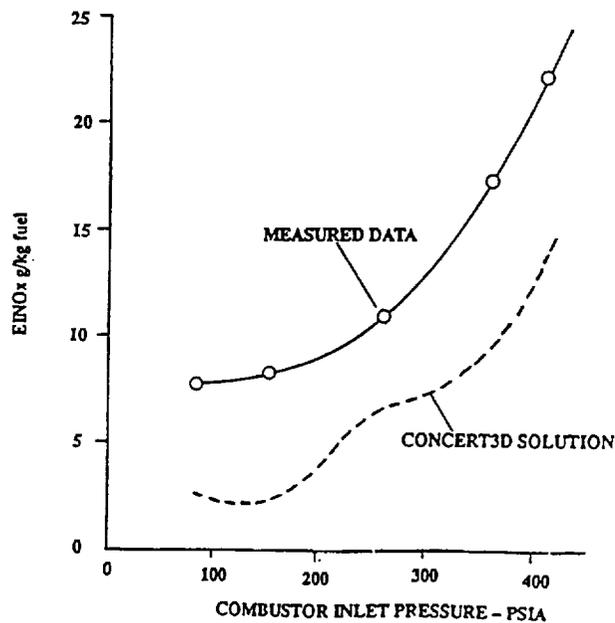
GAS TEMPERATURES (R)

CALCULATED FLOW FIELD IN PLANE IN LINE WITH SWIRLCUPS

CONCERT3D vs. RIG DATA COMPARISON FOR NASA/GE E3 COMBUSTOR
 (EXIT GAS TEMPERATURE AVERAGED AND MAXIMUM RADIAL PROFILES)



CONCERT3D vs. RIG DATA COMPARISON FOR NASA/GE E3 COMBUSTOR
 (NO_x EMISSIONS)



GEAE CONCERT EXPERIENCE:

CONCERT3D WITH PRESUMED SHAPE PDF/FAST CHEMISTRY MODEL AND THERMAL NO_x MODEL DOES WELL AGAINST REAL ENGINE DATA

CONCERT3D WITH TWO STEP EDDY BREAKUP MODEL DOES NOT CONSISTENTLY DEMONSTRATE ACCEPTABLE AGREEMENT FOR [CO] AND [HC] EMISSIONS

OTHER PERFORMANCE ISSUES NOT AS WELL PREDICTED COMPARED TO PRESUMED SHAPE PDF/FAST CHEMISTRY APPROACH

SHORTCOMINGS:

TWO STEP EDDY BREAKUP MODEL NOT ADEQUATE FOR THE REQUIRED LEVEL OF PREDICTIVE ACCURACY

FAST CHEMISTRY CANNOT PREDICT [CO], [HC], AND IGNITION, BLOWOUT, AND RELIGHT

REQUIRES ACCURATE FINITE RATE CHEMISTRY REPRESENTATION AND MORE ACCURATE TURBULENCE-CHEMISTRY INTERACTION MODELING

GE HAS EMBARKED ON THE DEVELOPMENT OF IMPROVED CONCERT MODELING CAPABILITIES

HYBRID CONCERT CFD / MONTE-CARLO MODELING APPROACH

APPROACH ADOPTED FOR THE NEXT RELEASE OF COMBUSTION CFD MODELING CAPABILITY AT GEAE

RETAINS;

- SINGLE STRUCTURED BODYFITTED GRID
- PRESSURE CORRECTION FINITE VOLUME FORMULATION
- K-E TURBULENCE MODELING WITH LOG WALL FUNCTIONS

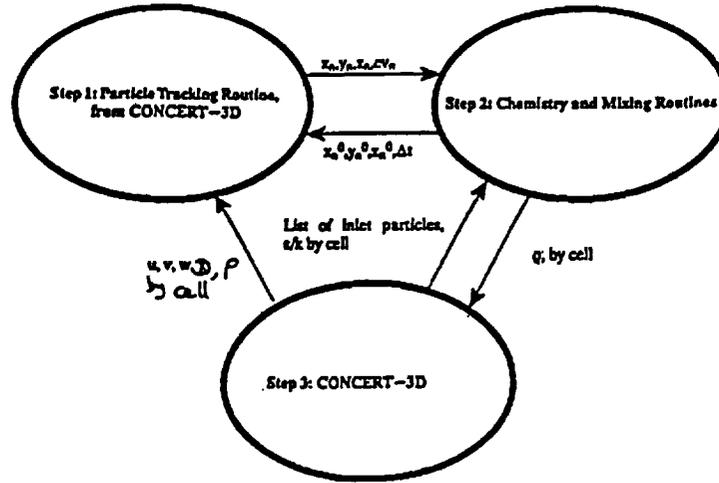
INTRODUCES;

- MONTE-CARLO SCALAR PDF TO ADDRESS TURBULENT COMBUSTION
 - SINGLE ATTRIBUTE (CONSERVED SCALAR) FOR FAST CHEMISTRY
 - MULTIPLE SCALARS FOR FINITE RATE CHEMISTRY OF CH₄ AND JETA FUELS BASED ON APPROPRIATE REDUCED MECHANISMS

DEVELOPMENT HAS BEEN UNDERWAY SINCE 1992

- 3D CODE DEVELOPMENT INITIATED IN MID YEAR 1993

HYBRID CONCERT CFD / MONTE-CARLO MODELING APPROACH



SCHEMATIC OF COMMUNICATIONS IN THE COMBINED CONCERT / MONTE-CARLO MODELING

HYBRID CONCERT CFD / MONTE-CARLO MODELING APPROACH

BETA TESTING INITIATED BEGINNING OF 1994

FOCUSED ON FAST CHEMISTRY CALCULATIONS AND OPTIMIZING COMPUTATIONAL EFFICIENCY

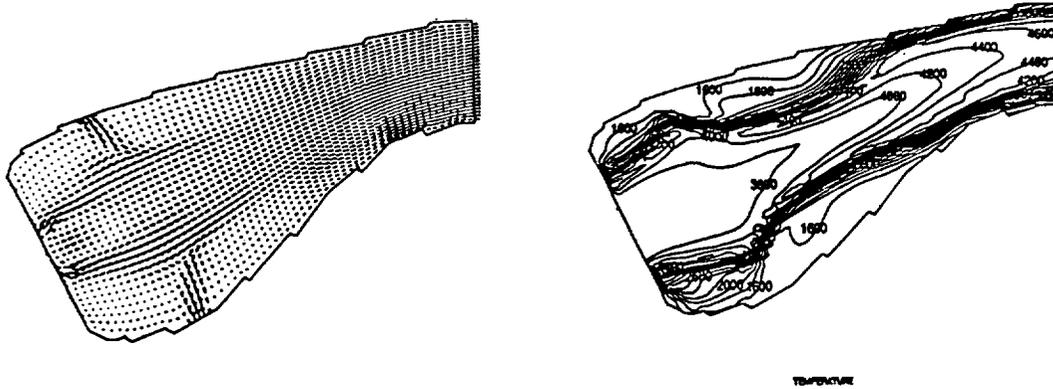
SIGNIFICANT IMPROVEMENT IN COMPUTATIONAL EFFICIENCY ACHIEVED

	TEST CASE 1	TEST CASE 2
NUMBER OF GRID POINTS	9,261	58,621
NUMBER OF M/C PARTICLES	216,000	1,500,000
CPU TIME (CRAY C-90 seconds)		
CONCERT WITHOUT M/C	83	5,400
INITIAL HYBRID CONCERT /MC	39,960	187,560
OPTIMIZED VERSION	1,770	41,400
PERCENT REDUCTION	-95.6%	-77.9%
WALL CLOCK TIMES (seconds) UTILIZING CRAY MULTI-TASKING OPTION	1,500	29,520

RUN TIMES HAVE BEEN REDUCED TO THE POINT WHERE OVERNIGHT TURNAROUND TIMES FOR A TYPICAL 3D COMBUSTOR MODEL ARE POSSIBLE

HYBRID CONCERT CFD / MONTE-CARLO MODELING APPROACH

(INITIAL 3D CALCULATION OF CFM56-3 COMBUSTOR WITH FAST CHEMISTRY)



CALCULATED FLOW FIELD IN PLANE IN LINE WITH INLET SWIRL CUPS

INITIAL CALCULATED RESULTS SHOW A TEMPERATURE FIELD THAT DOES NOT AGREE WELL WITH EXPECTED LEVELS. CALCULATION SHOWS CONSIDERABLY LESS DIFFUSION OF THE SCALAR FIELD (FUEL MIXTURE FRACTION) THAN OBSERVED FROM RIG DATA AND CONCERT CALCULATIONS PERFORMED USING THE PRESUMED SHAPE SCALAR PDF COMBUSTION MODELING APPROACH.

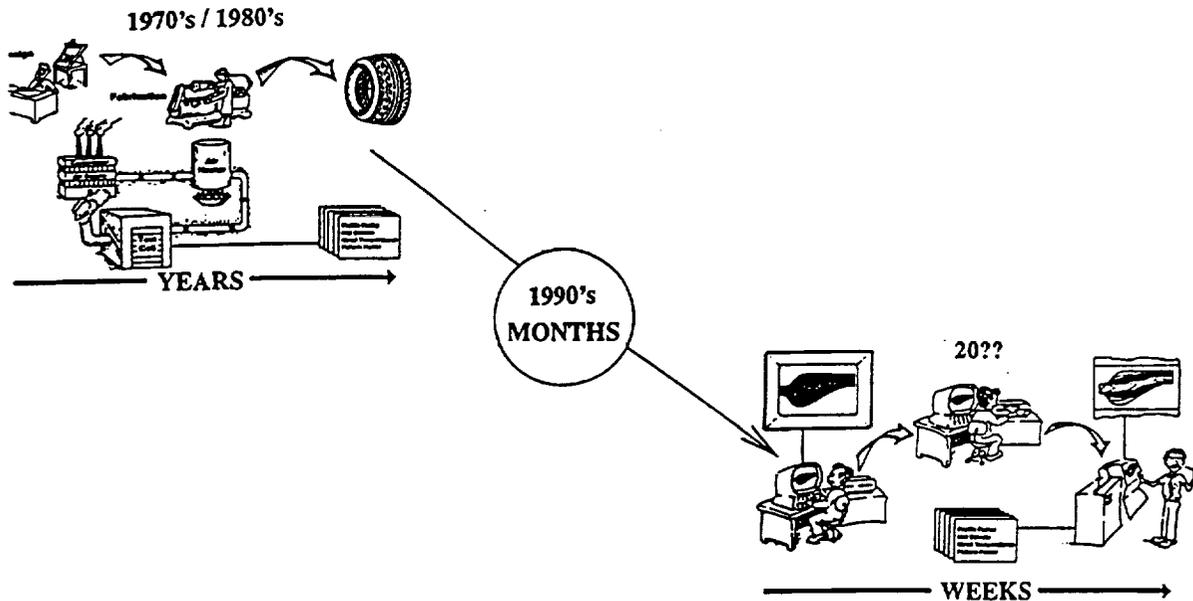
HYBRID CONCERT CFD / MONTE-CARLO MODELING APPROACH

FUTURE WORK PLANNED

- PERFORM CALCULATIONS AGAINST A BENCHMARK REACTING FLOW EXPERIMENT WITH AVAILABLE TEST DATA
 - BLUFF BODY STABILIZED FLAME ; (GULATI AND CORREA)
- SYSTEMATICALLY STUDY THE EFFECTS OF SCHMIDT NUMBER AND OTHER PARTICLE TRACKING PARAMETERS ON THE FAST CHEMISTRY SOLUTION TO IMPROVE AGREEMENT WITH THE DATA
- PERFORM 3D SINGLE AND DUAL ANNULAR COMBUSTOR CALCULATIONS AND COMPARE RESULTS WITH AVAILABLE GEAE DATA BASE
- IMPLEMENT REDUCED CHEMISTRY SCHEMES (MULTIPLE SCALARS) TO PERFORM FINITE RATE CHEMISTRY CALCULATIONS
 - PREDICT [CO], [HC], AND [NO_x] EMISSIONS
- RELEASE CODE FOR PRODUCTION USE AT GEAE
 - FAST CHEMISTRY BY END OF FIRST QUARTER OF 1995
 - FINITE RATE CHEMISTRY BY END OF THIRD QUARTER OF 1995

FUTURE MODELING DIRECTIONS

FOCUSED ON IMPROVING THE PREDICTIVE ACCURACY FOR ALL KEY COMBUSTOR PERFORMANCE ISSUES TO LEVELS THAT WOULD ELIMINATE THE NEED FOR COMPONENT RIG DEVELOPMENT TESTING



FUTURE MODELING DIRECTIONS

INDUSTRY WILL LOOK INCREASINGLY TO THE ACADEMIC COMMUNITY (UNIVERSITIES AND NATIONAL LABS) TO DEVELOP THE NEEDED MODELING IMPROVEMENTS

INDUSTRY MUST PROVIDE THE GUIDANCE AS TO WHAT IS NEEDED

FUTURE GENERATION MODELS MUST;

- PROVIDE MORE RIGOROUS REPRESENTATION OF COMPLEX PHYSICAL PROCESSES
- BE COST EFFECTIVE AS A ROUTINE APPLIED DESIGN/ANALYSIS TOOL
- RETAIN USER FRIENDLY CHARACTERISTICS
- PROVIDE THE LEVEL OF ACCURACY AND CAPABILITIES DEMANDED OF IT

COMPUTING PLATFORM CAPABILITIES ARE ADVANCING AT A RAPID PACE

THE PRACTICALITY OF ADVANCED MODELS IN INDUSTRY MAY NOT BE TOO FAR INTO THE FUTURE

TIME TO START NOW ON DEVELOPMENT OF THE ADVANCED MODELS OF THE FUTURE INTO PRACTICAL TOOLS TO HAVE THEM READY FOR USE WHEN THE REQUIRED COMPUTING PLATFORMS BECOME AVAILABLE IN INDUSTRY

Computational Turbulence 1994	1 ---- 6	Calculation of turbulent heat transfer in "cluttered spaces", by BRIAN SPALDING Topic 1: The WDIS & WGAP calculation.
<p>The need:</p> <ul style="list-style-type: none"> * Prandtl-mixing-length models require knowledge of distance from nearby walls AND between walls (eg Nikuradze formula) * Many low-Re models require the distance from nearby walls * In spaces "cluttered" with solids (eg electronics cooling), calculation of distances and gaps has, in the past, been time-consuming. <p>The solution:</p> <ul style="list-style-type: none"> * This contribution computes WDIS and WGAP (the required quantities) by solving: $\text{div grad } L = -1$ with L fixed to zero in solids. 		

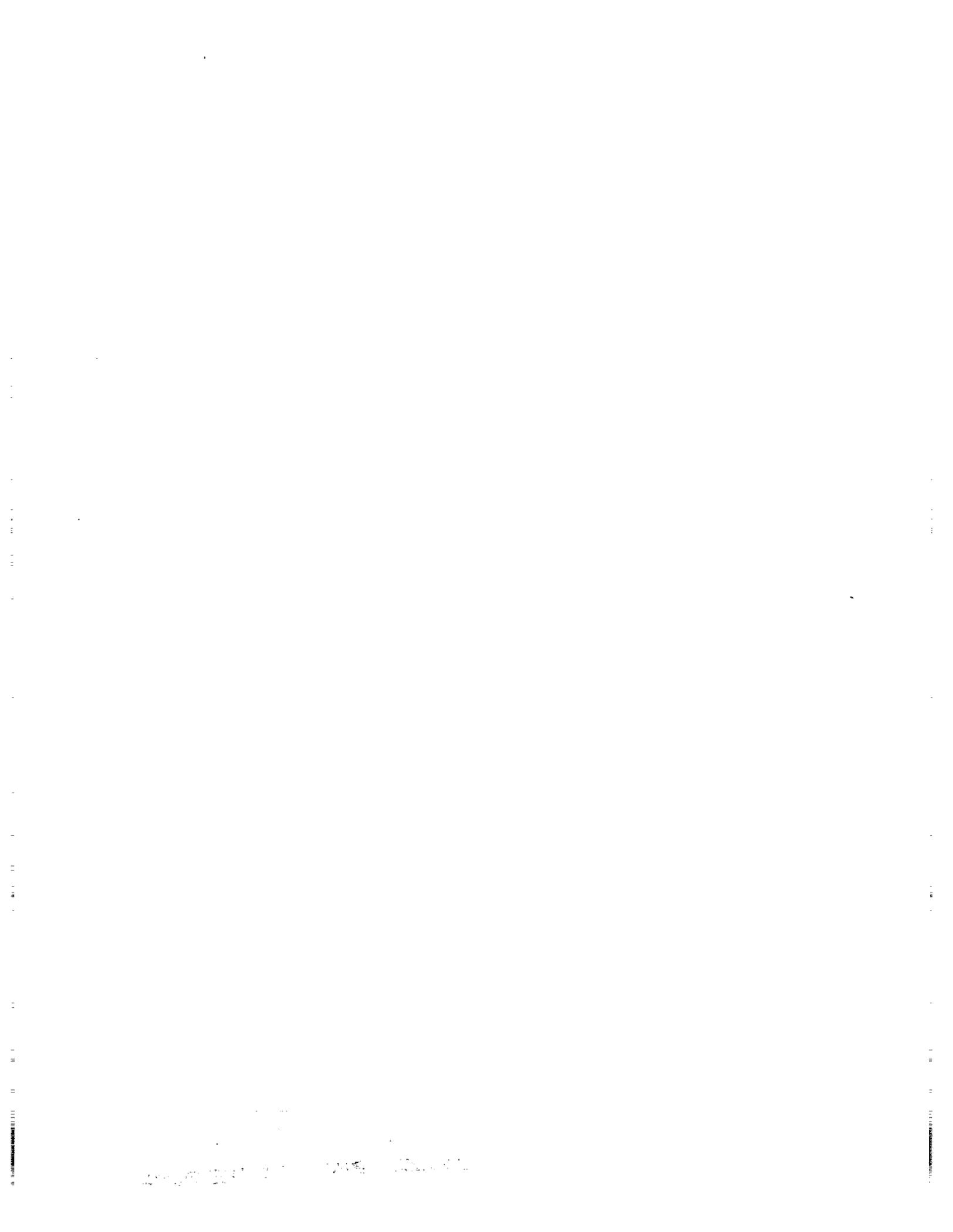
Computational Turbulence 1994	2 ---- 6	Outline of the theory
<p>Obviously L values which satisfy this equation will be proportional to the distance from the wall at points which are close to it. The question is: what is the proportionality constant?</p> <p>The constant depends also on the distance across the inter-solid space, which however is the other unknown which it is desired to determine.</p> <p>The practice adopted by the author is to deduce both the required quantities, WDIS the distance from the wall, and WGAP the distance between walls (whatever these quantities may mean in "cluttered spaces"), from the an algebraic fucntion of the local values of L and its gradient.</p>		

Computational Turbulence 1994	3 ---- 6	The results
<p>The formula employed gives exact results for situations where WDIS and WGAP have unequivocal meanings, namely for the space between two parallel plates or within a long circular-sectioned pipe; and it gives plausible results for more complex cases.</p> <p>The equation for L, with the appropriate boundary conditions, is of course very easy to solve by numerical means; so WDIS and WGAP can be quickly computed before the flow simulation starts.</p> <p>The use of the method is illustrated by a PHOENICS calculation for a geometry involving two boxes, a connecting arc, an inlet and an outlet. It was performed by I Poliakov and S Semin, of CHAM, to whom the author's thanks are due.</p>		

Computational Turbulence 1994	4 ---- 6	Calculation of turbulent heat transfer in "cluttered spaces", by BRIAN SPALDING Topic 2. The LVEL model.
<p>The need:</p> <ul style="list-style-type: none"> * In "cluttered" regions, the between-solid distances are too often too small for fine-grid resolution. * Reynolds numbers are usually low, at least in some places. * A model is needed which gives plausible results in these circumstances AND fits experimental data for better-studied ones. <p>The solution:</p> <ul style="list-style-type: none"> * The LVEL model of PHOENICS gets local effective viscosities from the analytical nu-plus-versus-u-plus relation which fits the laminar, transitional & full-turbulent ranges very well. Only local velocity and WDIS (wall distance) are needed. 		

Computational Turbulence 1994	5 ---- 6	Outline of the theory
<p>The u-plus versus y-plus formula of Spalding (1961) is employed namely:</p> $y^+ = u^+ + (1/E) * [\exp(K^*u^+) - 1 - K^*u^+ - (K^*u^+)^{**2}/2 - (K^*u^+)^{**3}/6 - (K^*u^+)^{**4}/24]$ <p>which implies the formula for dimensionless effective viscosity:</p> $v^+ = 1 + (K/E) * [\exp(K^*u^+) - 1 - K^*u^+ - (K^*u^+)^{**2}/2 - (K^*u^+)^{**3}/6]$ <p>With the wall-distance and the velocity known at every point, the effective viscosity can also be computed at every point.</p> <p>The method is valid for the whole range of Reynolds numbers; but it is best supplemented by a low-Re "v+-collapse" formula.</p>		

Computational Turbulence 1994	6 ---- 6	The results
<p>The LVEL model gives the well-known experimental results for simple circumstances, such as flow in pipes and between parallel plates; and it gives plausible results for more complex cases.</p> <p>The use of the method is illustrated by a PHOENICS calculation of the flow and heat transfer in a small part of a large space cluttered with solids which participate in the heat-transfer process.</p> <p>The method is the only plausible and practicable one known to the author for handling heat transfer in electronics-cooling problems, because of the excessive grid-fineness requirements of low-Reynolds-number k-epsilon extensions.</p>		



RECENT PROGRESS IN THE JOINT VELOCITY-SCALAR PDF METHOD

M.S. Anand
Allison Engine Company
Indianapolis, Indiana

N95- 27890

- o TURBULENCE
- o REACTION (treatment, kinetic schemes, emissions)
- o TURBULENCE/CHEMISTRY INTERACTIONS
- o ATOMIZATION
- o SPRAY EVAPORATION

SIMULATION ISSUES:

- o NUMERICS (accuracy, convergence)
- o GEOMETRY (body-fitted grids, unstructured grids)
- o COMPUTATIONAL RESOURCES (Time, Storage)

JOINT VELOCITY-SCALAR PDF METHOD

SIGNIFICANT MILESTONES AND RECENT PROGRESS

- o 2-D and 3-D time dependent flows (with finite-volume method)
(Anand et al. 1987, Haworth & El Tahry 1989)
- o Stochastic dissipation model development and validation
(Pope & Chen 1990, Pope 1991, Anand et al. 1993)
- o 2-D Elliptic flows (mean pressure algorithm), swirling flows
(Anand et. 1989, 1993)
- o Spray treatment
(Anand 1990)
- o Manifold methods for reaction kinetics
(Maas & Pope 1992, 1994; Norris & Pope 1994; Norris & Hsu 1994)

- o Solve Poisson equation for mean pressure:

$$\frac{\partial^2 \langle p \rangle}{\partial x_j \partial x_j} = - \frac{\partial^2}{\partial x_i \partial x_j} \langle \rho U_i U_j \rangle$$

- o Satisfy continuity by solving for velocity correction potential, velocity correction:

$$\frac{\partial^2 \phi}{\partial x_i \partial x_i} = - \frac{\partial}{\partial x_i} \langle \rho U_i \rangle \quad ; \quad \Delta U_i = \frac{1}{\langle \rho \rangle} \frac{\partial \phi}{\partial x_i}$$

- o Solution algorithm is consistent with B-spline representation of mean fields

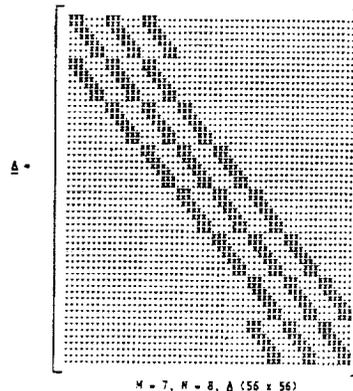
- o Same discretized form: $\underline{\underline{A}} \cdot \underline{\underline{s}} = \underline{\underline{b}}$

- o $\underline{\underline{A}}$ is a banded matrix, constant and same for both $\langle p \rangle$ and ϕ

- o LU decomposition only once

- o Special band solver economizes storage and computational effort

- o Judicious implementation of the algorithm results in significant economy in computer resource requirement



TURBULENT COMBUSTION MODELING ISSUES

(FOR GAS TURBINE COMBUSTORS)

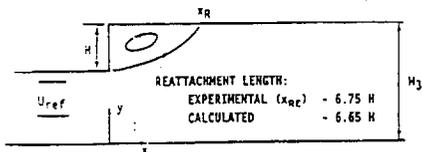
o Most promising method for turbulent reacting flows

ATTRIBUTES OF DIFFERENT PDF METHODS

<u>Method</u>	<u>Attributes</u>	<u>Limitations/shortcomings</u>
Joint PDF of ϕ	Reaction treated exactly	Assumes gradient-diffusion, Does not give velocity field (requires e.g. $k-\epsilon$) Turbulence/chemistry interactions not fully simulated
Joint PDF of \underline{U} and ϕ	Reaction exact, Convection (mean and turbulent) exact, Variable-density effects exact	Needs ϵ equation (or equivalent)
Joint PDF of \underline{U} , ϕ , and ω	... In addition Provides complete closure, Treats turbulent streams of different scales, Can account for effects of large scale structures	

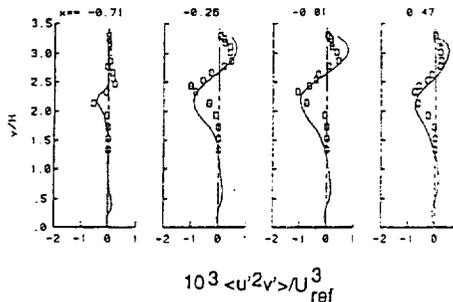
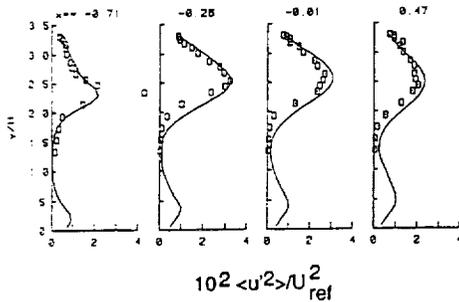
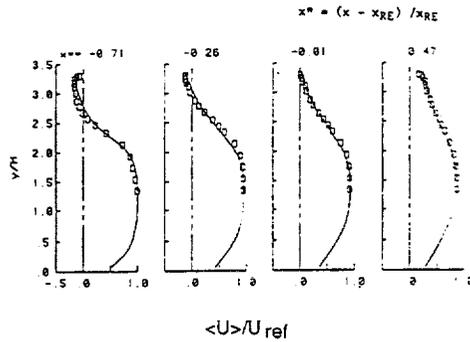
PDF CALCULATIONS FOR A RECIRCULATING FLOW

(Anand et al. 1989)



Backward-facing step
Pronchick and Kline (1983)

Storage: 1.3 Mwords
CPU Time: 6 min. Cray YMP



STOCHASTIC DISSIPATION MODEL

- o Provides complete closure of the PDF equation (joint velocity-frequency-scalar)
- o More realistic than a mean dissipation model. Dissipation (rather, turbulent frequency) is also a random variable and included in the joint PDF.
- o Treats multiple scales in the flow
- o Accounts for internal intermittency
- o Accounts for effects of large scale structures, and influence of origin and history of the fluid particles

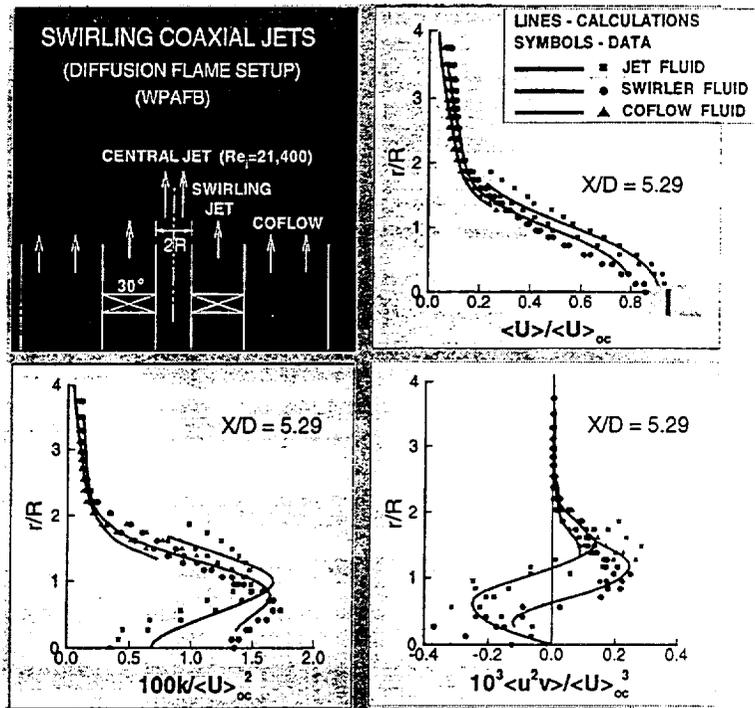
$$d\omega^* = -\omega^* \langle \omega \rangle (S_\omega + C_\chi \Omega) dt + \langle \omega \rangle^2 h dt + \omega^* (2C_\chi \langle \omega \rangle \sigma^2)^{1/2} dW$$

$$dU_i^* = -\frac{1}{\rho} \frac{\partial \langle P \rangle}{\partial x_i} dt + D_i dt + (C_o \bar{k} \omega^*)^{1/2} dW_i$$

SWIRLING FLOWS

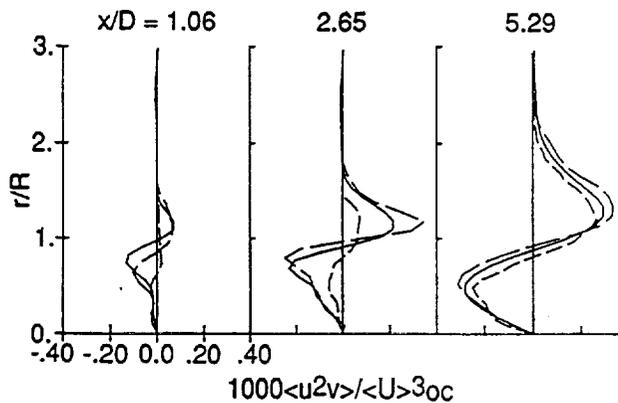
- o No theoretical limitations
- o Additional production terms due to non-zero mean swirl velocity
- o Additional terms in calculating the mean pressure (or mean pressure gradients)
 - Boundary layer flows:
 - > radial pressure gradient
 - > axial pressure gradient also included
 - Elliptic flows
 - > additional terms in the Poisson equation for pressure
- o Validation of the stochastic dissipation model and first calculation of swirling flows with the joint PDF method (Anand et al. 1993)

JOINT PDF CALCULATIONS FOR SWIRLING FLOWS



JOINT PDF CALCULATIONS FOR SWIRLING FLOWS

COMPARISON WITH REYNOLDS-STRESS MODEL RESULTS AND
ASSESSMENT OF GRADIENT DIFFUSION MODELING



RS MODEL:

$$\langle u^2v \rangle = -C_s \frac{k}{\langle \epsilon \rangle} \langle v^2 \rangle \frac{\partial \langle u^2 \rangle}{\partial r}$$

$$C_s = 0.22$$

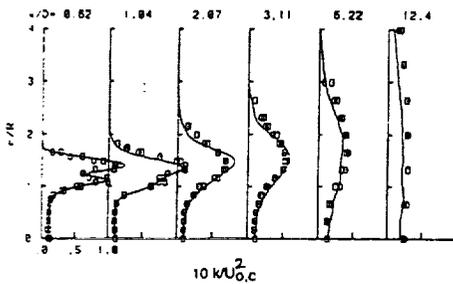
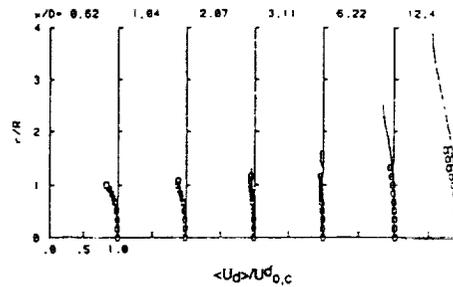
— PDF CALCULATIONS
- - - RS MODEL WITH RSM RESULTS
· · · RS MODEL WITH PDF RESULTS

SPRAY CALCULATIONS

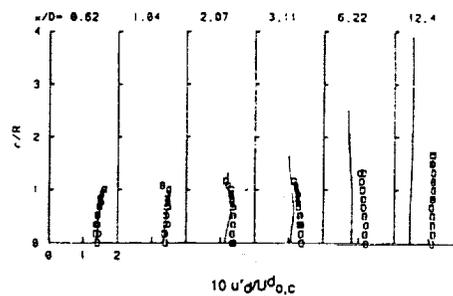
(Anand 1990)

- o Advanced spray models (stochastic Lagrangian, Monte Carlo) naturally compatible with the joint PDF method
- o Assumptions about turbulent kinetic energy partition avoided
- o Effects of gas phase turbulence structure (velocity cross-correlation) included

105 micron glass beads, NASA HOST C data

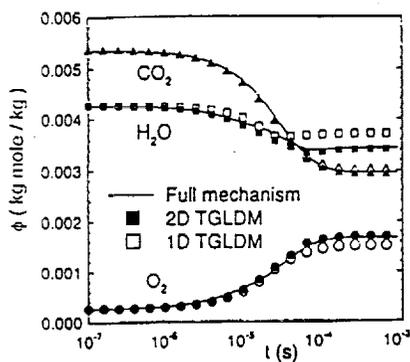


Computed profiles of normalized turbulent kinetic energy of air compared against data.

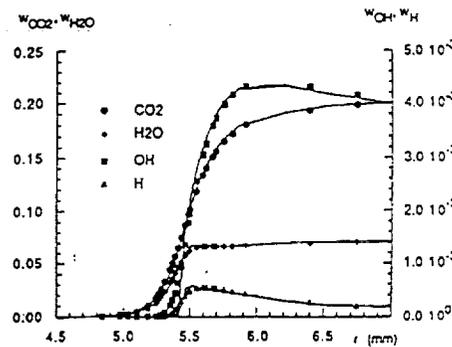


REDUCED KINETICS / MANIFOLD METHODS

- o Low dimensional manifold methods (ILDM, TGLDM)
 - Given detailed kinetics, they provide low-dimensional description (e.g., 1-D, 2-D, 3-D) in multidimensional composition/scalar space
 - Use dynamical systems theory to determine the low. dim. manifold
 - Avoid ad hoc assumptions, e.g, partial equilibrium of some of the reactions
Implications for ignition and lean blow-off
 - Not fuel specific like conventional reduced kinetic schemes



Perfectly Stirred Reactor (Pope & Maas 1993)



Laminar Premixed Flame (Maas & Pope 1994)

PARALLEL PROCESSING

- o Objective: Turnaround time of 1 day or less for 3-D combustor calculations
 - o Particle partitioning, domain decomposition (multigrid, multi-block)
 - o Preliminary results for 2-D flow with particle partitioning (Pope 1994)
 - 16 nodes, 128 MB each, IBM SP1
 - 12.8 million particles (800,000 per processor)
 - 50 time steps
 - 44 minutes/processor (45 minutes clock time)
- Extrapolation to 3-D combustor calculations
- 6.5 hours clock time with 32 processor SP1

JOINT PDF FOCUS AREAS

- o 3-D Flows, Improved solution algorithms
- o Parallel processing
- o Reduced kinetics / Low Dimensional Manifolds
- o Evaporating / reacting sprays
- o Emphasis on emissions and performance predictions

**OVERVIEW OF TURBULENCE MODEL DEVELOPMENT AND
APPLICATIONS AT ROCKETDYNE**

N95- 27891

**A.H. Hadid, E.D. Lynch, and M.M. Sindir
Rocketdyne Division
Rockwell International
Canoga Park, California**

**TURBULENCE MODELING REQUIREMENTS,
DEVELOPMENT PHILOSOPHY AND APPROACH**

- **REQUIREMENTS**
 - TURBULENCE MODELING IS A KEY ENABLING TECHNOLOGY FOR ALL PROPULSION RELATED CFD ACTIVITIES
 - FACTORS TO CONSIDER INCLUDE ACCURACY, CONSISTENCY, COMPUTATIONAL COST, AND EASE OF USE
 - TURBULENCE MODELS THAT CAN NOT BE INCLUDED IN PRODUCTION GRADE CFD CODES ARE OF LIMITED VALUE TO INDUSTRY
- **PHILOSOPHY**
 - BASIC MODEL DEVELOPMENT IS BEST LEFT TO SPECIALIZED "CENTERS OF EXCELLENCE"
 - VARIOUS CLASSES OF MODELS NEED TO BE SUPPORTED SINCE NO SINGLE UNIVERSAL MODEL IS SHOWN TO EXIST
 - ESTABLISHING THE RANGE OF APPLICABILITY, ACCURACY, AND THE COMPUTATIONAL COST OF THE MODELS IS ESSENTIAL

**TURBULENCE MODELING REQUIREMENTS,
DEVELOPMENT PHILOSOPHY AND APPROACH (Cont.)**

- **APPROACH**
 - IDENTIFY KEY "CENTERS OF EXCELLENCE" AND ESTABLISH COLLABORATIVE RELATIONSHIP
 - ACQUIRE MODELS AND ASSESS PERFORMANCE FOR THE INTENDED CLASS OF APPLICATIONS
 - DELINEATE MODEL DEFICIENCIES AND INITIATE EFFORT TO REDUCE THEM
 - DEVELOP MODELS INTO STAND-ALONE MODULES
 - INCLUDE MODULES IN PRODUCTION CODES AND ESTABLISH BASELINE FOR APPLICATIONS

TWO MAJOR AREAS OF CONCENTRATION

- **HIGH SPEED TURBULENCE MODELING (LEAD DR. DOUG LYNCH)**
 - FOCUSED ON HIGH SPEED ($M > 1$) PROPULSION (ROCKET AND AIRBREATHING) AND AERODYNAMICS
 - EMPHASIS ON 2-EQUATION PHENOMENOLOGICAL MODELS WITH NASA ARC AND LARC AS KEY TECHNOLOGY PARTNERS
 - LES WORK IN PLANNING STAGES WITH CTR
- **LOW SPEED TURBULENCE MODELING (LEAD DR. ALI HADID)**
 - FOCUSED ON LOW SPEED ($M < 1$) AND ROTATING FLOW APPLICATIONS
 - EMPHASIS ON REYNOLDS STRESS PHENOMENOLOGICAL MODELS IN COLLABORATION WITH UMIST, ICOMP, CTR, AND UAH
 - LES WORK INITIATED WITH CTR

HIGH SPEED TURBULENCE MODELING

- **EMPHASIS IS ON THE DEVELOPMENT OF ENGINEERING TURBULENCE MODELS FOR**
 - HIGH SPEED AIRBREATHING PROPULSION SYSTEMS
 - THRUST CHAMBERS
 - VEHICLE AERODYNAMICS
- **APPROACH TAKEN IS BASED ON 2-EQUATION MODELS**
 - DIFFERENT CLASSES OF 2-EQUATION MODELS STUDIED
 - $k-\epsilon$
 - $k-\omega$
 - POINTWISE R_f
 - COMPRESSIBILITY EFFECTS AND TURBULENCE-CHEMISTRY INTERACTIONS MAJOR MODEL UPGRADE THRUSTS
 - COMPRESSIBILITY MODIFICATIONS FROM ARC
 - TURBULENCE-CHEMISTRY INTERACTION MODELS FROM LARC
 - **USA AND GASP SERVE AS NUMERICAL PLATFORM**
 - **GASP** - CHIEN, LAM-BREMHORST $k-\epsilon$, $k-\omega$
 - **USA** - VARIETY OF $k-\epsilon$, $k-\omega$

COMPRESSIBILITY EFFECTS

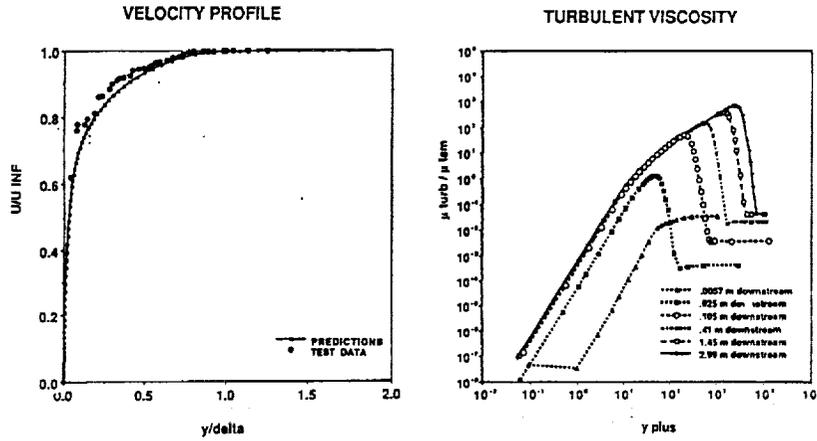
- MIXING LAYER SPREADING REDUCED AT HIGH MACH NUMBERS
 - INCREASE DISSIPATION RATE OF k
 - DEFINE Ck_2 AS A FUNCTION OF TURBULENT MACH NUMBER $\sqrt{\rho k/\gamma p}$
 - ZEMAN MODIFICATION (1990)
 - SARKAR (1990, 1991) AND WILCOX (1991) PROPOSALS
 - MODIFICATIONS OF ZEMAN AND SARKAR NOT RECOMMENDED
- HEAT TRANSFER OVER PREDICTED NEAR SHOCK WAVES
 - LIMIT TURBULENT LENGTH SCALE L_t TO $\min\left(\frac{k^{3/2}}{\epsilon}, \frac{Ky}{C\mu^{3/4}}\right)$ (VUONG AND COAKLEY, 1987)
- SEPARATION UNDERPREDICTED IN RAPID COMPRESSION OR STRAIN REGIONS
 - INCREASE α_ϵ OR α_ω UNDER RAPID COMPRESSION (VUONG AND COAKLEY)
- HEAT TRANSFER OVER PREDICTED FOR VERY COLD WALLS $T_w/T_{aw} < 0.1$ (COAKLEY)
 - CEBECI-SMITH ~ 60%, $k-\omega$ ~ 40%, $q-\omega$ ~ 10%, $k-\epsilon$ ~ 30%

TURBULENCE MODELS ADAPTED TO USA CODE

ALGEBRAIC	DAMPING		BOUNDARY CONDITIONS	TRANSITION MODEL		COMPRESSIBILITY EFFECTS		
	WALL	LOCAL		HIGH ORDER POLYNOMIAL	ARNAL	MIXING LAYER SPREADING	SEPARATION EXTENT	REATTACHMENT HEAT TRANSFER
Baldwin-Lomax	X	3 Versions		X	X			
$k-\epsilon$								
1. Myong-Kasagi	X	X	$k=0$ $\epsilon = \nu \mu^2 \gamma^2$	X		1. Sarkar (1991) 2. Zeman (1990) 3. Wilcox (1991)	4. Yuong & Coakley (1987)	5. Yuong & Coakley (1987)
2. Chien (1982)	X	X	$k=0$ $\epsilon=0$	X		1., 2., 3.	4.	5.
3. Jones-Launder (1972)	X	X	$k=0$ $\epsilon=0$	X		1., 2., 3.	4.	5.
4. Launder-Sharma (1974)	X	X	$k=0$ $\epsilon=0$	X		1., 2., 3.	4.	5.
5. Huang-Coakley (1992)	X	X	$k=0$ $\epsilon = 2\nu\mu k_1 \gamma^2$	X		1., 2., 3.	4.	5.
6. Speziale-So-Zhang (1993)	X	X	$k=0$ $\epsilon = 2\nu\mu k_1 \gamma^2$	X		1., 2., 3.	4.	5.
7. Lam-Bremhorst (1981)	X	X	$k=0$ $\epsilon_y=0$	X		1., 2., 3.	4.	5.
8. High Re	X	X	Wall Function	X				
$k-\omega$								
1. High Re Wilcox (1991a)	-	-	$k=0$ $\omega_0 = 10\omega_1$	X		1., 2., 3.	4.	5.
2. Low Re Wilcox (1991b)	-	-	$k=0$ $\omega = 7.2\nu\mu \gamma^2$	X		1., 2., 3.	4.	5.
$q-\omega$								
Coakley (1987)			$k=0$ $\omega_y=0$	X				
One-Equation (Goldberg, - Two-Time Scale 1992)			$k=0$					
One-Equation R_T (Goldberg 1993, 1994)		X	$\frac{d(\frac{k^2}{\epsilon})}{dy} = \frac{d(\nu_1 R_T)}{dy} = 0$	X				

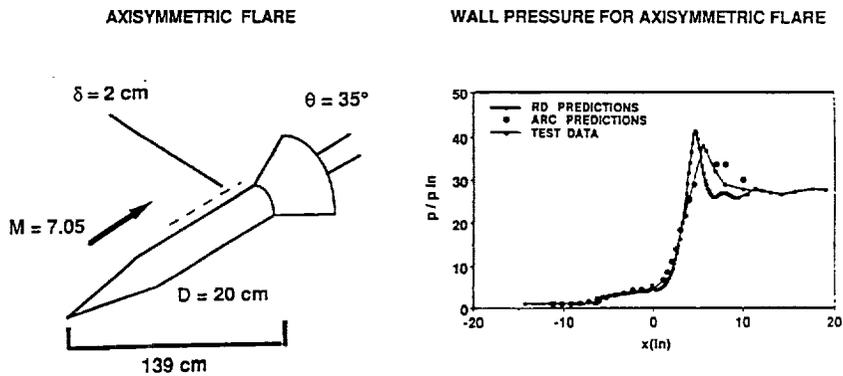
M = 9.2 FLAT PLATE FLOW

- CHIEN $k-\epsilon$ MODEL WITH RAPID COMPRESSION AND LENGTH SCALE COMPRESSIBILITY MODIFICATIONS



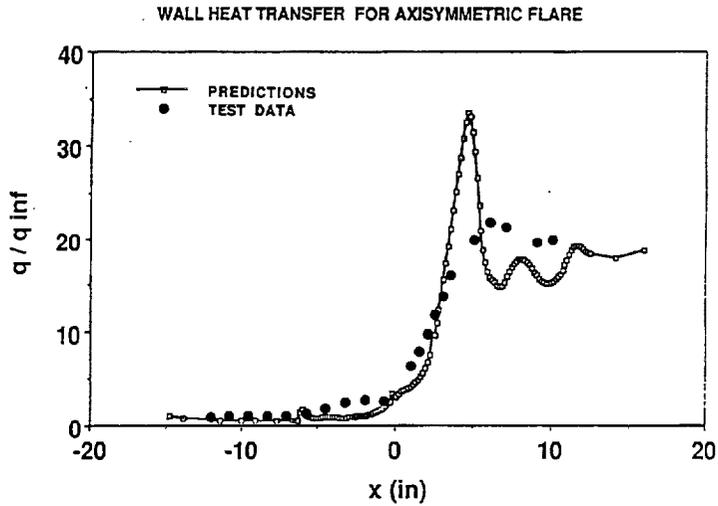
REF: G.T. COLEMAN AND J.L. STOLLERY, JFM 56: 741, "HEAT TRANSFER FROM A HYPERSONIC TURBULENT FLOW AT A WEDGE COMPRESSION CORNER"

MACH 7.05 FLOW OVER AXISYMMETRIC FLARE CHIEN $k-\omega$ MODEL WITH RAPID COMPRESSION AND LENGTH SCALE COMPRESSIBILITY MODIFICATIONS



REF: M.I. KUSSOY AND C.C. HORSTMAN, "DOCUMENTATION OF TWO- AND THREE-DIMENSIONAL HYPERSONIC SHOCK-WAVE TURBULENT BOUNDARY LAYER INTERACTION FLOW," NASA TM 1-01075.

MACH 7.05 FLOW OVER AXISYMMETRIC FLARE
CHIEN $k-\omega$ MODEL WITH RAPID COMPRESSION AND LENGTH SCALE
COMPRESSIBILITY MODIFICATIONS



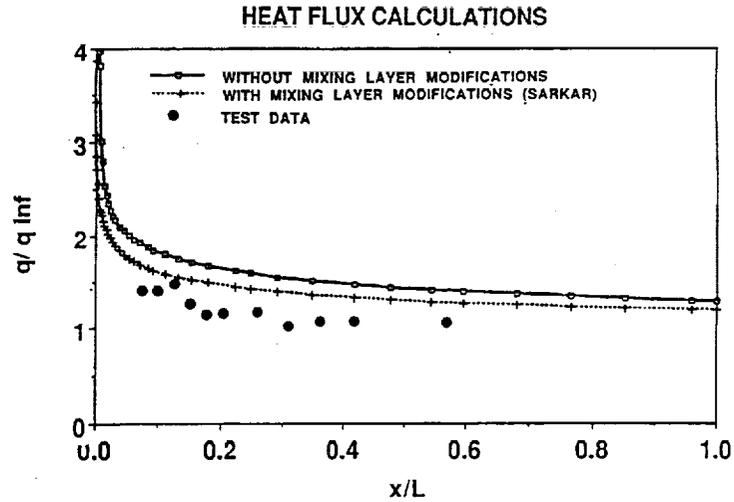
MACH 8.6 FLOW OVER COLD WALL WEDGE



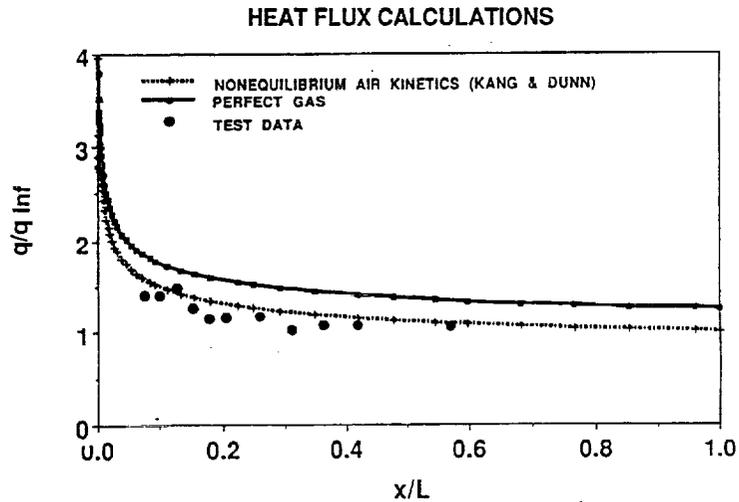
THREE STUDIES

1. CHIEN $k-\epsilon$ MODEL WITH RAPID COMPRESSION AND LENGTH SCALE CORRECTIONS AND WITH AND WITHOUT MIXING LAYER TREATMENT
2. HIGH- Re $k-\omega$ MODEL WITH VARIOUS AIR CHEMISTRY MODELS
3. BALDWIN-LOMAX TURBULENCE MODEL USING WALL AND LOCAL DAMPING

MACH 8.6 FLOW OVER COLD WALL WEDGE
CHIEN k-ε MODEL WITH AND WITHOUT MIXING LAYER TREATMENT

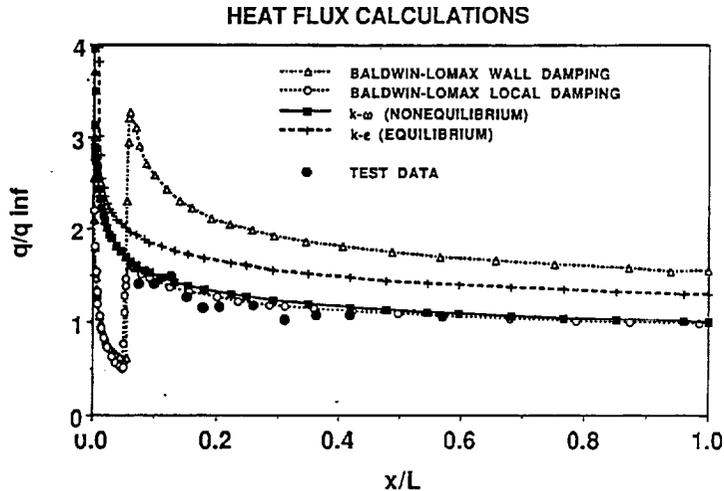


MACH 8.6 FLOW OVER COLD WALL WEDGE
HIGH-Re k-ω MODEL WITH VARIOUS AIR CHEMISTRY MODELS



MACH 8.6 FLOW OVER COLD WALL WEDGE

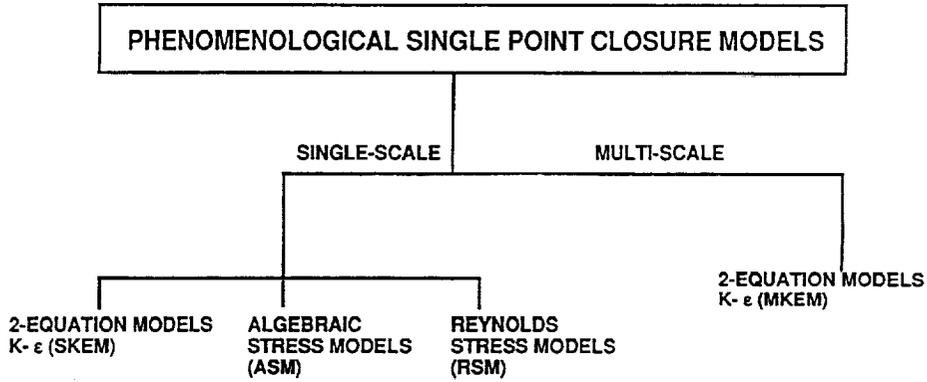
BALDWIN LOMAX, $k-\epsilon$, $k-\omega$ MODEL COMPARISONS



LOW SPEED TURBULENCE MODELING

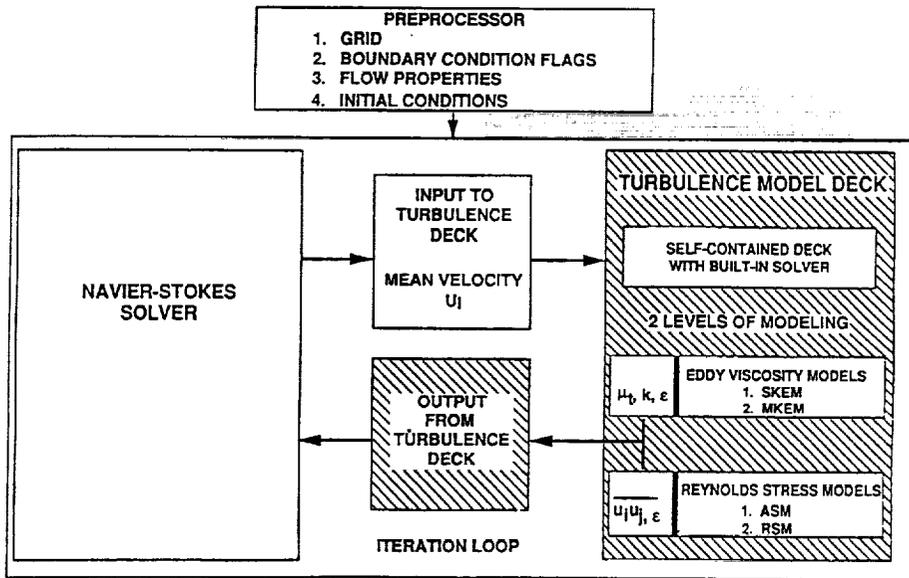
- EMPHASIS IS ON THE DEVELOPMENT OF ENGINEERING TURBULENCE MODELS FOR
 - ROTATING MACHINERY
 - FLOW IN DUCTS AND MANIFOLDS
 - REACTING FLOWS
- APPROACH TAKEN IS TO
 1. SYSTEMATICALLY ASSESS EXISTING PHENOMENOLOGICAL MODELS USING COMMON NAVIER-STOKES SOLVER
 2. IDENTIFY, DEVELOP AND VALIDATE MODEL UPGRADES COMMENSURATE WITH OBSERVED FLOWPHYSICS
 3. DEVELOP SELF-CONTAINED TURBULENCE MODEL DECKS (MODULES) THAT CAN BE INTEGRATED WITH NAVIER-STOKES SOLVERS
 4. PROVIDE GUIDANCE TO EXPERIMENTAL AND THEORETICAL RESEARCH IN TURBULENCE MODELING FOR ENGINEERING APPLICATIONS

TURBULENCE MODELS BEING ASSESSED



NEAR-WALL TREATMENTS INCLUDE (WHERE APPROPRIATE) WALL FUNCTIONS, MULTILAYER MODELS, AND LOW-REYNOLDS NUMBER APPROXIMATIONS

TURBULENCE MODEL DECK STRUCTURE AND INTEGRATION WITH NAVIER-STOKES SOLVER



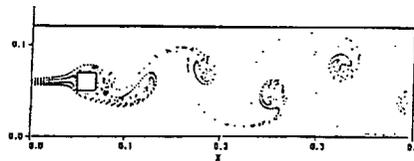
PROJECT WELL UNDERWAY

- **TEAM**
 - MODELS PROVIDED BY UMIST, LERC/ICOMP, ARC/CTR
 - MODULE DEVELOPMENT BY ROCKETDYNE
 - MODULE TESTING BY ROCKETDYNE (REACT, USA) AND UAH (MAST)
 - MODEL UPGRADES BY ROCKETDYNE, UMIST, ARC/CTR
 - APPLICATION BY ROCKETDYNE TO TURBOPUMP COMPONENT (E.G. IMPELLER) ANALYSIS
- **2-D MODULES COMPLETED, TESTED, AND RELEASED**
 - SINGLE SCALE $k-\epsilon$
 - MULTI SCALE $k-\epsilon$
 - ASM
 - RSM
- **3-D MODULE DEVELOPMENT IN PROGRESS**

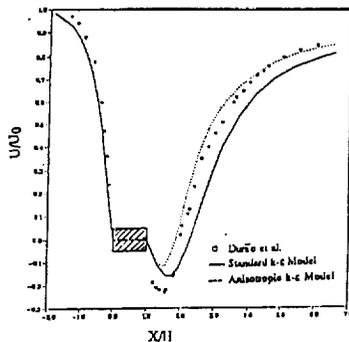
NONLINEAR ALGEBRAIC-STRESS MODEL

VORTEX SHEDDING FROM RECTANGULAR CYLINDERS (DURAO, et al)

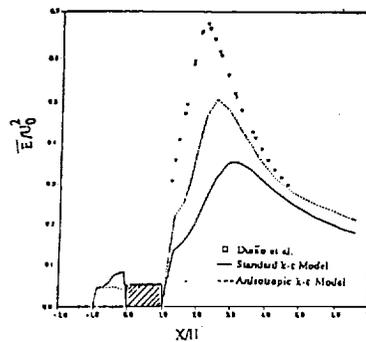
PARTICLE STREAKLINES



MEAN AXIAL VELOCITY ALONG CENTERLINE

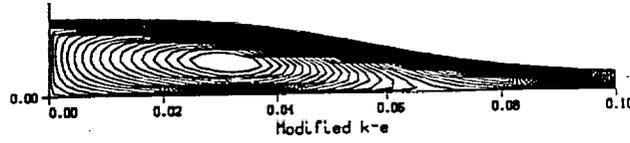


MEAN KINETIC ENERGY ALONG CENTERLINE

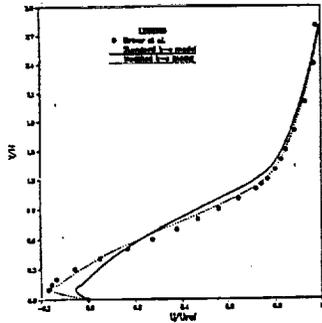


ROTATION MODIFIED k-ε MODEL BACKWARD FACING STEP (DRIVER AND SEEGMILLER)

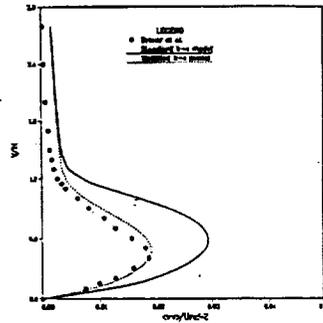
STREAMLINE CONTOURS



MEAN AXIAL VELOCITY AT X/M=4

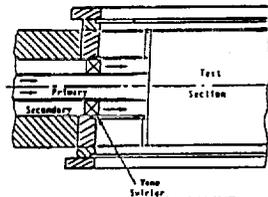


RADIAL TURBULENT INTENSITY ($\sqrt{v'v'}/u_{ref}^2$)

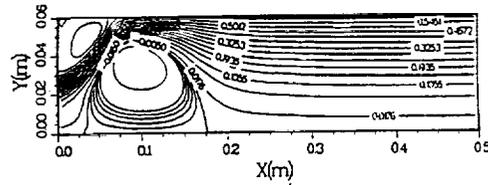


ALGEBRAIC STRESS MODEL CONFINED COAXIAL SWIRLING JET FLOW (ROBACK AND JOHNSON)

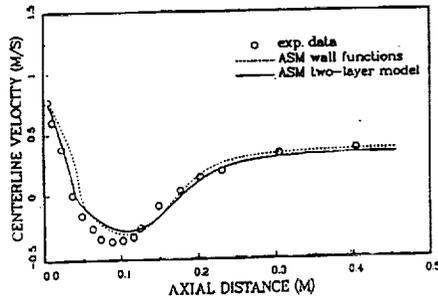
GEOMETRY



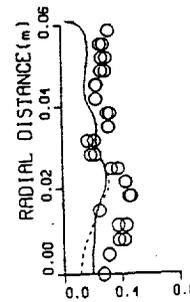
STREAMLINE CONTOURS



DECAY OF MEAN AXIAL CENTERLINE VELOCITY



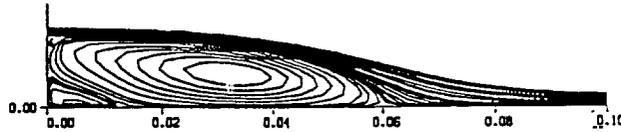
RADIAL PROFILES OF $\overline{u'u'}$
25 mm



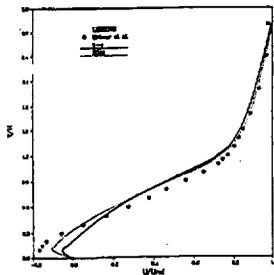
REYNOLDS STRESS MODEL (LRR – MODEL)

BACKWARD FACING STEP (DRIVER AND SEEGMILLER)

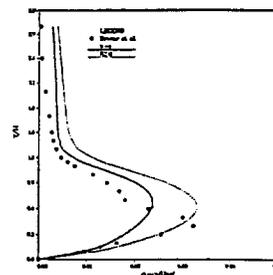
STREAMLINE CONTOURS



MEAN AXIAL VELOCITY AT X/H=4



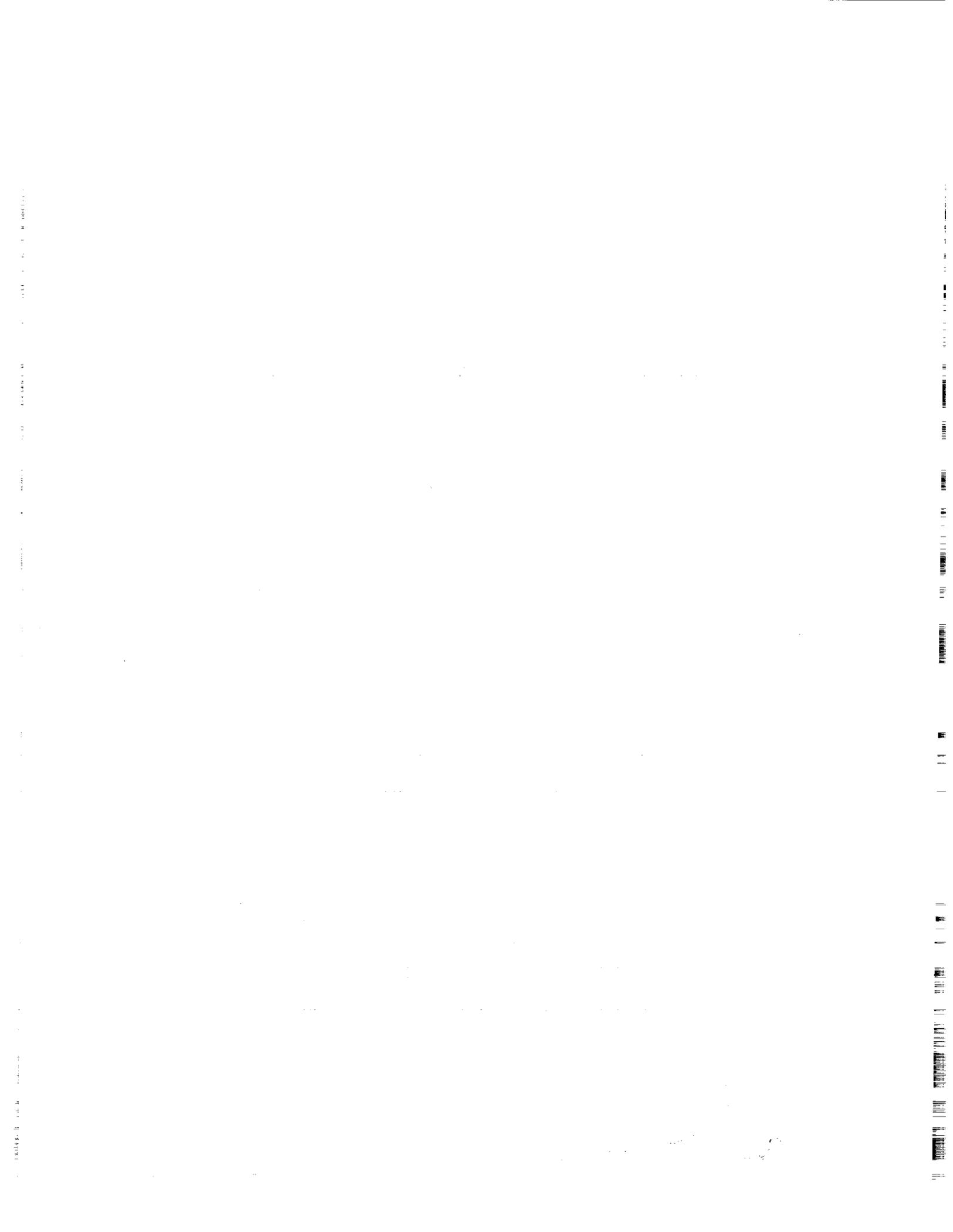
AXIAL TURBULENCE INTENSITY AT X/H=4



CONCLUDING REMARKS

- PROGRAMS (BOTH COMMERCIAL AND GOVERNMENT) EMPLOY NEW TECHNOLOGY ONLY WHEN IT PROVIDES "ADDED VALUE"
 - REDUCED DEVELOPMENT COST
 - INCREASED RELIABILITY AND PERFORMANCE
 - ENHANCED MANUFACTURABILITY
- THE NEW TECHNOLOGY WE OFFER IS THE COMPUTATIONAL ENGINEERING TOOLS FOR PRODUCT DESIGN AND ANALYSIS
- THESE TOOLS ARE THE END PRODUCT FOR ALL ENABLING TECHNOLOGY DEVELOPMENT
 - PRE- AND POST PROCESSING
 - ALGORITHMS AND NUMERICAL PLATFORMS
 - PHYSICAL MODELS (E.G. TURBULENCE AND CHEMISTRY)
- FAILURE OF ANY ENABLING TECHNOLOGY JEOPARDIZES THE PERFORMANCE (VALUE) OF THE TOOL

NOW MORE THAN EVER, THERE IS A NEED FOR CLOSER COLLABORATION AND COOPERATION BETWEEN GOVERNMENT, INDUSTRY, AND RESEARCH INSTITUTIONS TO ENSURE MAINTENANCE OF COUNTRY'S TECHNOLOGY BASE



A.D. Leonard and F. Dai
CFD Research Corporation
Huntsville, Alabama

N95- 27892

ACKNOWLEDGEMENTS

- **NASA LeRC - Phase II SBIR**
Technical Monitor: David Fricker
- **Pratt & Whitney: Dr. Geoff Sturgess**
- **Wright Laboratories: Mr. Dale Shouse**

MOTIVATION

Accurate and Efficient Prediction of Emissions

- 1. Accurate Prediction of Emissions From Combustion Devices Requires Treatment of Finite-Rate Kinetics**
- 2. The Effect of Turbulent Fluctuations in Velocity, Energy, Composition, etc. on Finite-Rate Chemical Kinetics Must be Modeled**

TURBULENCE/CHEMISTRY INTERACTIONS

Possible Approaches

- **Neglect Fluctuations**
 - + **Simple**
 - **Ignores Effect of Turbulence**
- **Eddy Break Up**
 - + **Simple**
 - **Assumes Fast Chemistry**
 - **Mean Density, Temperature Must Still Be Modeled**
- **Prescribed PDF**
 - + **Efficient**
 - **Limited to Fast Chemistry or Single Step Reaction**
- **Composition PDF**
 - + **Finite-Rate Multi-Step Kinetics**
 - **Expensive**
 - **Gradient Diffusion**
- **Velocity-Composition PDF**
 - + **More Accurate**
 - **More Expensive**

PARTICLE REPRESENTATION

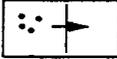
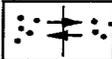
A Solution Method for a Large Number of Independent Variables

- **Computational Requirements Increases Exponentially With Dimensions for Finite Difference Methods**
- **Computational Requirements Increase Linearly With Dimensions for Monte Carlo Methods**

COMPOSITION PDF SOLUTION

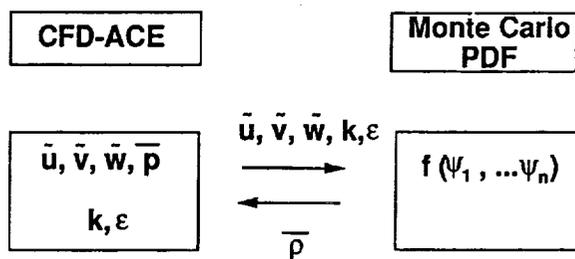
Stochastic Lagrangian Particle Simulation

Particle Composition and Position Changed to Model Transport of Joint PDF

- **Mean Convection**
 - Move Particles Between Cells 
- **Chemical Reactions**
 - Lookup Table Holds Composition Change
- **Turbulent Diffusion**
 - Exchange Particles Between Cells 
- **Molecular Mixing**
 - Particle Interaction Changes Composition

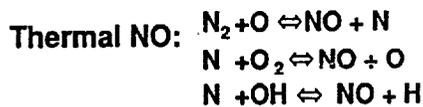
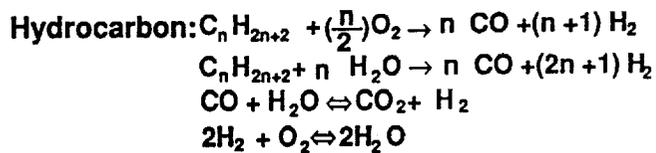
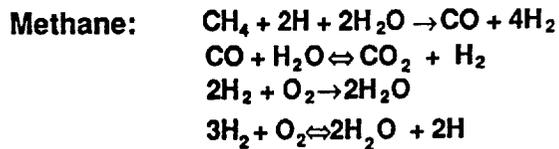
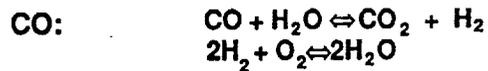
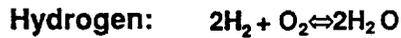
COUPLING

PDF Solution is Separate Module



CHEMICAL KINETICS

Reduced Models are Used

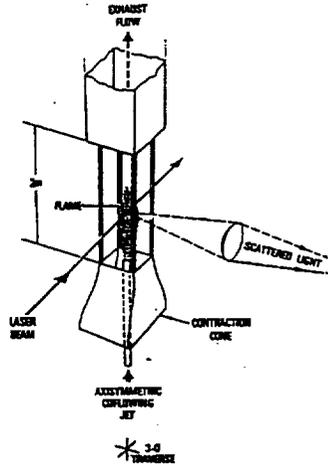


RESULTS TO BE PRESENTED

- Jet Diffusion Flame (Hydrogen with Helium Dilution)
- Bluff Body Stabilized Flame (H_2/CO)
- Piloted Jet Diffusion Flame (Methane)
- Generic Gas Turbine Combustor (Propane)

HYDROGEN JET DIFFUSION FLAME

Illustration of Experiment at Sandia National Lab



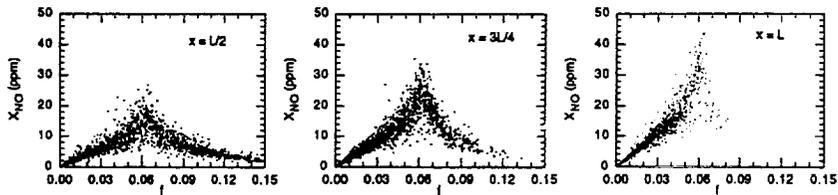
$Re \approx 10^4$

Fuel

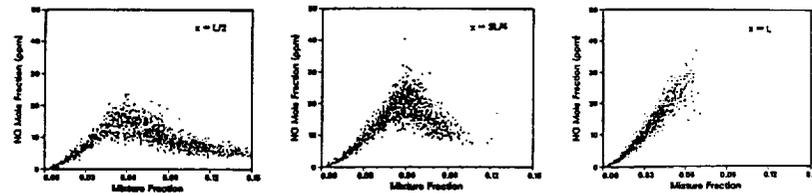
100% H₂
 80% H₂, 20% He
 60% H₂, 40% He

60% HYDROGEN FLAME

Scatter Plots of Mixture Fraction and NO Mole Fraction



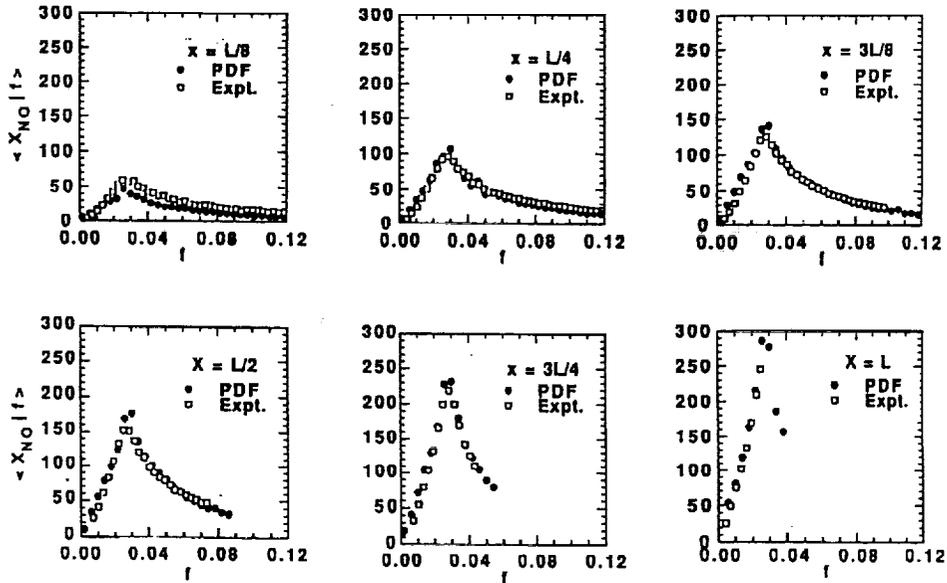
PDF Results



Experime Data

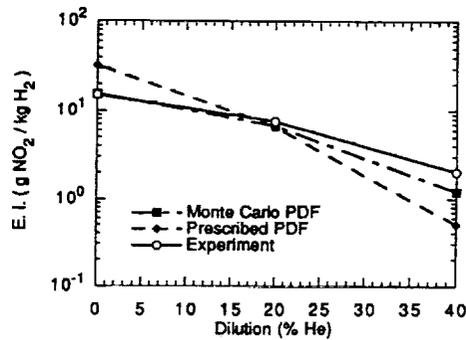
UNDILUTED HYDROGEN FLAME

Conditional Averged NO Mole Fraction



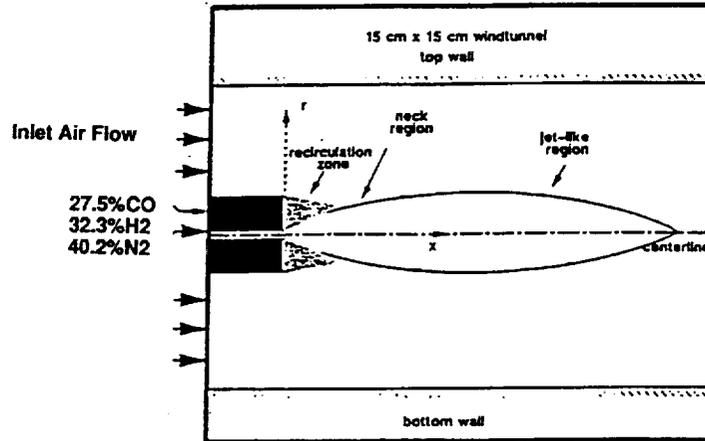
HYDROGEN DIFFUSION FLAME

Dilution Effects on Emmissions Index



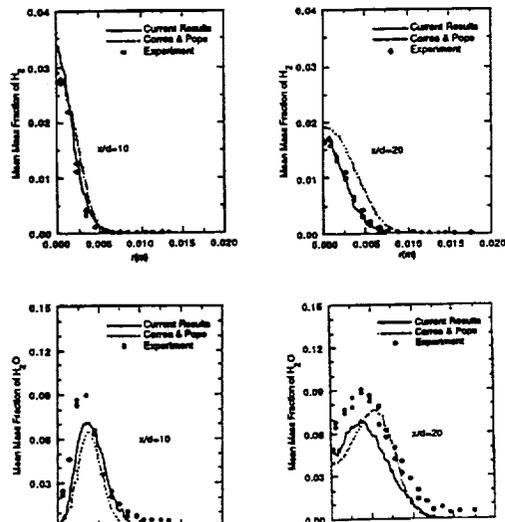
BLUFF BODY STABILIZED DIFFUSION FLAME

Illustration of Experiment of Corréa and Gulati



BLUFF BODY STABILIZED DIFFUSION FLAME

Composition PDF Predicts Mean Values as well as Velocity-Composition PDF

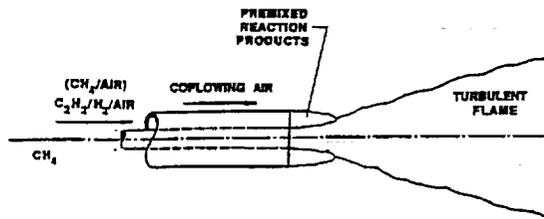


PILOTED JET DIFFUSION FLAME

Illustration of Experiment of Masri et.al.

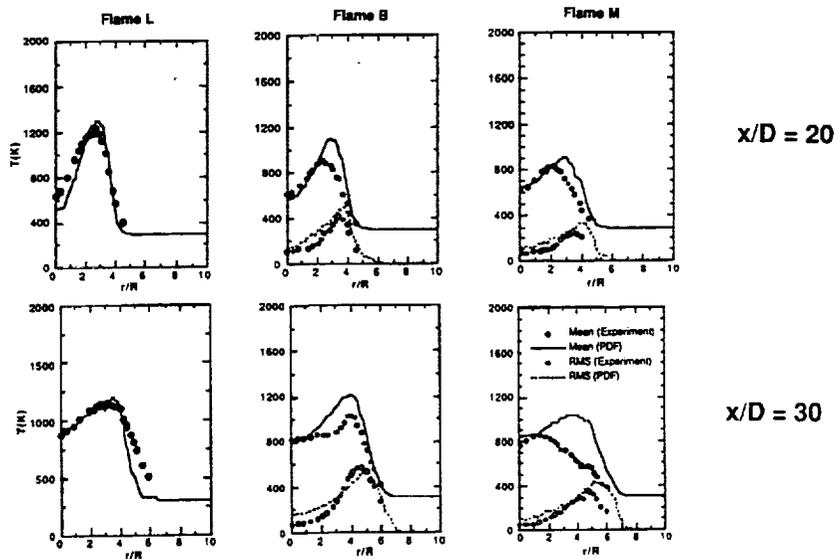
Experimental Conditions

Flame	Fuel Jet Velocity
L	41 m/s
B	48 m/s
M	55 m/s

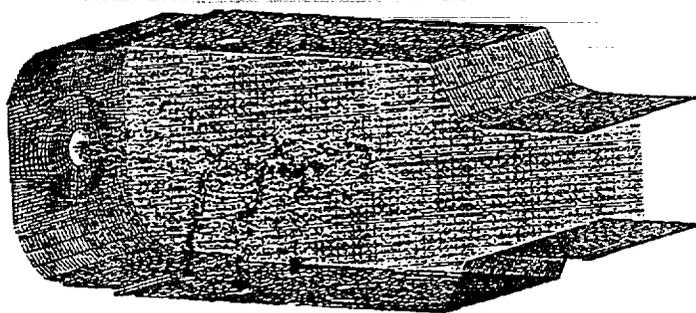


PILOTED JET DIFFUSION FLAME

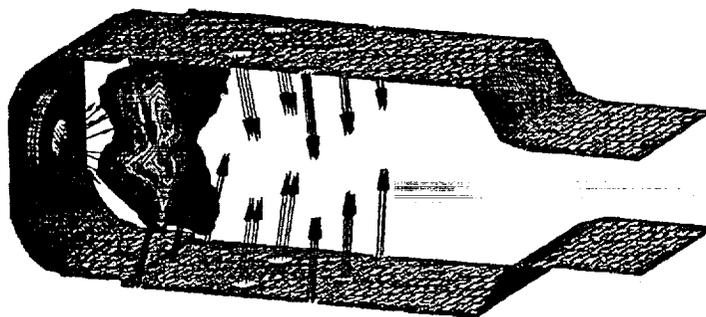
Good Agreement with Experimental Data



MONTE CARLO PDF COMBUSTOR CALCULATION
Stochastic Particle Traces



VERTICAL PLANE THROUGH CENTER OF
FUEL INJECTOR
Mean CO Mass Fraction Countours



RUN TIME AND MEMORY

3D Combustor Calculation (68,000 cells)

Conventional CFD

CPU Time	20 hours
Memory	80 MBytes

Monte Carlo PDF

CPU Time	100 hours
Memory	120 MBytes

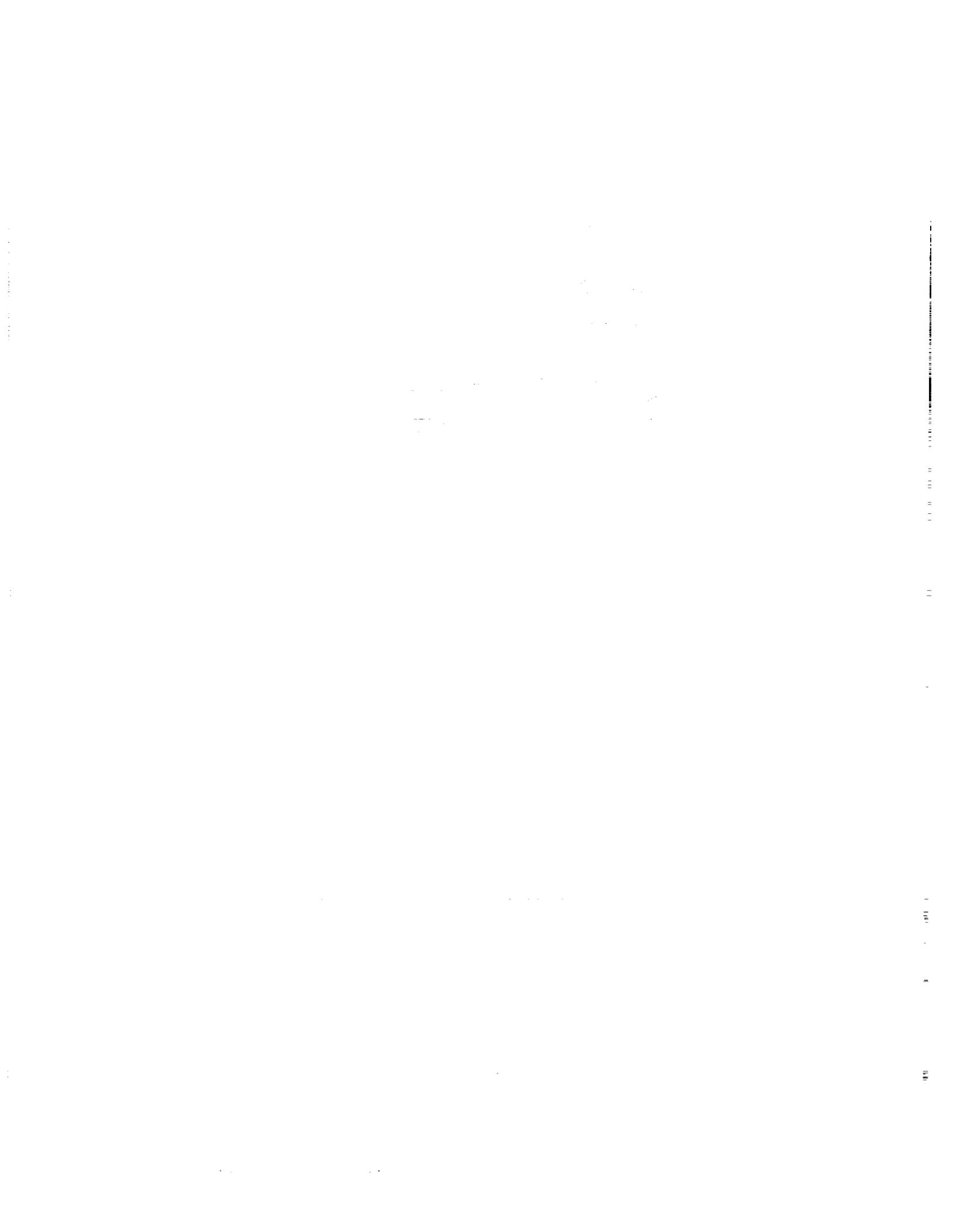
Parallel PDF (Projected)

CPU Time	25 hours	25 hours	25 hours	25 hours
Memory	30 MBytes	30 MBytes	30 MBytes	30 MBytes

CPU Time for IBM RS/6000 Model 560

CONCLUSIONS

- **Monte Carlo PDF Solution Successfully Coupled with Existing Finite Volume Code**
 - **Minor Changes to Finite-Volume Code**
 - **Can be Coupled with Other Codes**
- **PDF Solution Method Applied to Turbulent Reacting Flows**
 - **Good Agreement with Data for 2D Case**
 - **Demonstration of 3D Elliptic Flow**
- **PDF Methods Must be Run on Parallel Machines for Practical Use**



D. Choudhury, S.E. Kim, D.P. Tselepidakis,
and M. Missaghi
Fluent Inc.
Lebanon, New Hampshire

Outline of Talk

- Part I: Turbulence Modeling
 - Challenges in Turbulence Modeling
 - Desirable Attributes of Turbulence Models
 - Turbulence Models in FLUENT
 - Examples using FLUENT
- Part II: Combustion Modeling
 - Turbulence-Chemistry Interaction
 - FLUENT Equilibrium Model
- Concluding Remarks

Part I: Turbulence Modeling and Industrial Flows

- Many industrial flows are turbulent; certainly in the markets that two of our codes, FLUENT and RAMPANT, are focused in.
- Turbulence augments rates of mass, momentum and heat transfer, often by orders of magnitude.
- Most combustion processes involve turbulence and often depend on it.
- Choice of turbulence model dictates the accuracy of CFD predictions.
- There is still a large gap between the state-of-the-art and users' expectations and needs.

Challenges in Turbulence Modeling

- Modeling the correlations: $\overline{\rho u_i u_j}$ and $\overline{\rho u_i \phi}$.
 - Closures based on the “eddy-viscosity” concept (industry’s most popular choice)
 - Closures based on transport equations (RSM)
- Modeling an additional transport equation for a scalar quantity to fix the state of turbulence.
 - Most popular choice: the kinetic energy dissipation rate, ϵ .
 - However, this equation is derived by continuum mechanics-based phenomenological considerations and intuition.
- Modeling of the viscosity-affected, near-wall laminar sublayer.
 - Most popular choice: “Wall-functions” that bridge the turbulent field to the solid wall.
 - However, assumptions involved are not always right.

Desirable Attributes of Turbulence Models in Commercial CFD Codes

- Accuracy and Universality
 - The range of applicability should be as broad as possible.
 - Applicable to complex geometries and unstructured meshes.
- Economy
 - Mathematically simple.
 - Memory and CPU requirements should be moderate and affordable (model formulation and grid distribution requirements).
- Robustness
 - Model should be able to solve a wide range of problems with little or no convergence problems.
 - Computationally efficient (fast execution speed and uses memory sparingly).

Turbulence Models in FLUENT

- k - ϵ model adequate for simple flows with no significant strain rates.
- RNG k - ϵ model for separated flows, flows with large streamline curvature, swirling flows, or flows with significant strain rates.
- RSM recommended for swirling flows or highly anisotropic flows.

k - ϵ Model: Some Comments

- Well-tested, used for over 20 years, limitations well understood.
- It forms a good compromise between universality and economy of use for many engineering problems.
- Subject to the inherent limitations of the Boussinesq's hypothesis, i.e., isotropic eddy-viscosity and Newtonian closure (gradient-diffusion model).
- Many assumptions are introduced in deriving the modeled equations for the turbulent quantities, particularly the ϵ -equation, making their fidelity limited.
- The constants in the modeled equations are calibrated against simple benchmark experiments.
- As a result, the k - ϵ model performs poorly in flows with curvature, swirl, rotation, separated flows, low-Reynolds number flows, strongly anisotropic flows, etc.

Renormalization Group (RNG) Based k - ϵ Model

- Basic theory and derivation are described in Yakhot and Orszag (1986). Further details and applications are in Yakhot, Orszag, Thangam, Speziale, and Gatski (1992), Speziale and Thangam (1992).
- First introduced in a commercial code, FLUENT, in 1992.
- The RNG method is essentially a scale-elimination technique that can be applicable to the Navier-Stokes and other scalar transport equations as well.
- Removal of successively large scales leads to differential transport equation models and associated formula for quantities such as the turbulent Prandtl/Schmidt number.
- The basic form of the RNG-based k - ϵ equations remains largely the same with the standard k - ϵ model. But, the constants in the model equations are derived explicitly from theory.
- The ϵ -equation ends up with an additional source term, a strain-dependent term.
- The RNG model can be integrated directly to a solid wall without using *ad hoc* damping functions or damping terms used in many near-wall models.
- High-Re form of the turbulence kinetic energy and dissipation rate equations derived by RNG procedure are:

$$\begin{aligned}\frac{\partial k}{\partial t} + U_i \frac{\partial k}{\partial x_i} &= P_k - \epsilon + \frac{\partial}{\partial x_i} \left(\nu_T \frac{\partial k}{\partial x_i} \right) \\ \frac{\partial \epsilon}{\partial t} + U_i \frac{\partial \epsilon}{\partial x_i} &= 1.42 \frac{\epsilon}{k} P_k - 1.68 \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_i} \left(\frac{\nu_T}{\sigma_\epsilon} \frac{\partial \epsilon}{\partial x_i} \right) - \mathfrak{R}\end{aligned}$$

where:

$$\sigma_k = \sigma_\epsilon = 0.7179$$

$$P_k = 2\nu_T S_{ij} S_{ij} \text{ is the kinetic energy production}$$

$$S_{ij} = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \text{ is the mean rate of strain tensor}$$

$$\nu_T = C_\mu \frac{k^2}{\epsilon}$$

$$\mathfrak{R} = \frac{C_\mu \eta^3 (1 - \frac{\eta}{\eta_0})}{1 + \beta \eta^3} \frac{\epsilon^2}{k}$$

$$\eta = Sk/\epsilon, \quad S = (2 S_{ij} S_{ij})^{1/2}$$

$$\eta_0 = 4.38, \quad \beta = 0.015$$

RNG-Based k - ϵ Model (Cont'd)

- In the low-Re RNG model, a differential relationship exists between $\frac{k}{\sqrt{\epsilon}}$ and ν_{eff} (Yakhot and Orszag, 1986).
- The turbulent Prandtl/Schmidt number is no longer a constant, and computed from relationships relating the local value of the number to the viscosity ratio (Yakhot and Orszag, 1986).
- In these relations, as $\hat{\nu} \rightarrow 1$, $\alpha \rightarrow \alpha_0$ (the low-Re limit) and as $\hat{\nu} \rightarrow \infty$, $\sigma = \alpha^{-1} \rightarrow 0.7179$ (the high-Re limit). Here:
 $\hat{\nu} = \nu_{\text{eff}}/\nu_0$, where $\nu_{\text{eff}} = \nu_0 + \nu_T$
 $\alpha =$ inverse turbulent Prandtl number (σ^{-1})
 $\alpha_0 =$ inverse molecular Prandtl number (σ_0^{-1})

- In the low-Re regions, σ_k and σ_ϵ are obtained similarly from the Prandtl number relationships, with $\alpha_0 = 1.0$.
- The relationships ensure that in the high-Re number part of the flow where $\hat{\nu} \gg 1$:

$$\nu_{\text{eff}} = \nu_T = 0.085 \frac{k^2}{\epsilon}$$

and the effective viscosity varies smoothly from the molecular viscosity to the turbulent viscosity.

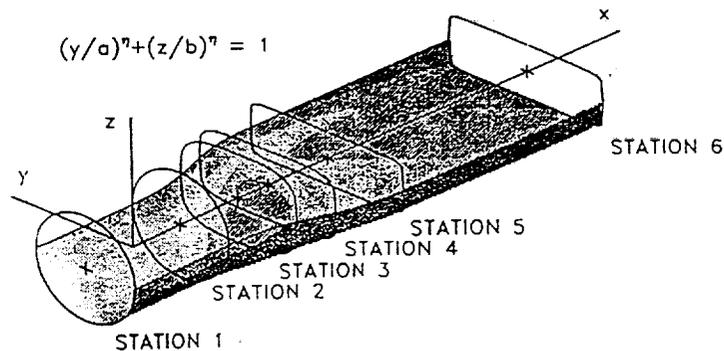
- The low-Re eddy-viscosity formula does not explicitly involve any geometric length scale, i.e., the distance from a solid wall used in the damping functions adopted by most low-Re near-wall models, which is a very convenient feature for calculations for complex three-dimensional geometries.
- In collaboration with the originators of the RNG model, Drs. Yakhot and Orszag, the model has been extended to account for the effects of compressibility, swirl, rotation, and premixed combustion.
- The RNG-based k - ϵ model also works well with conventional and enhanced (non-equilibrium) wall functions available in Fluent Inc.codes.

The Reynolds-Stress Model in FLUENT

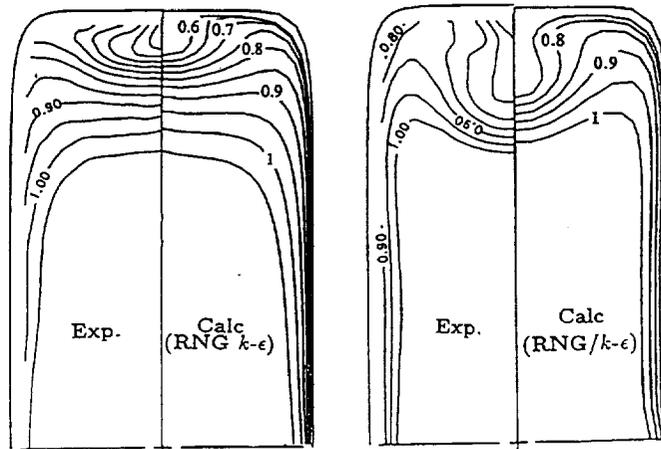
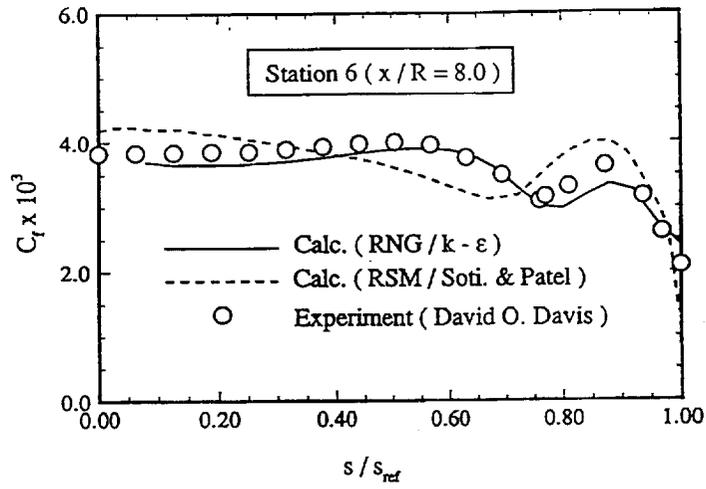
- RSM solves transport equations for the Reynolds stresses: $\overline{u_i u_j}$, (4 equations in 2D problems, 6 equations in 3D problems).
- RSM is the level of modeling that has a well established track record of out-performing eddy-viscosity models in complex flows.
- It is computationally more expensive and more inclined to divergence and stability problems.
- The simple and most widely tested form of the Launder, Reece and Rodi (1975) form is used.
- The interpolation technique for co-located grids of Rhie and Chow (1983) is used.
- It offers the best choice for highly anisotropic flows.

Example 1: Circle-to-Rectangle Transition Duct

- Measured by Davis (1991).
- $Re_D = 3.9 \times 10^5$.
- Solution Domain.
 - Upstream Inlet Boundary: $x/D = -1.0$
 - Downstream Exit Boundary: $x/D = 8.0$
 - A Quadrant of the duct modeled.



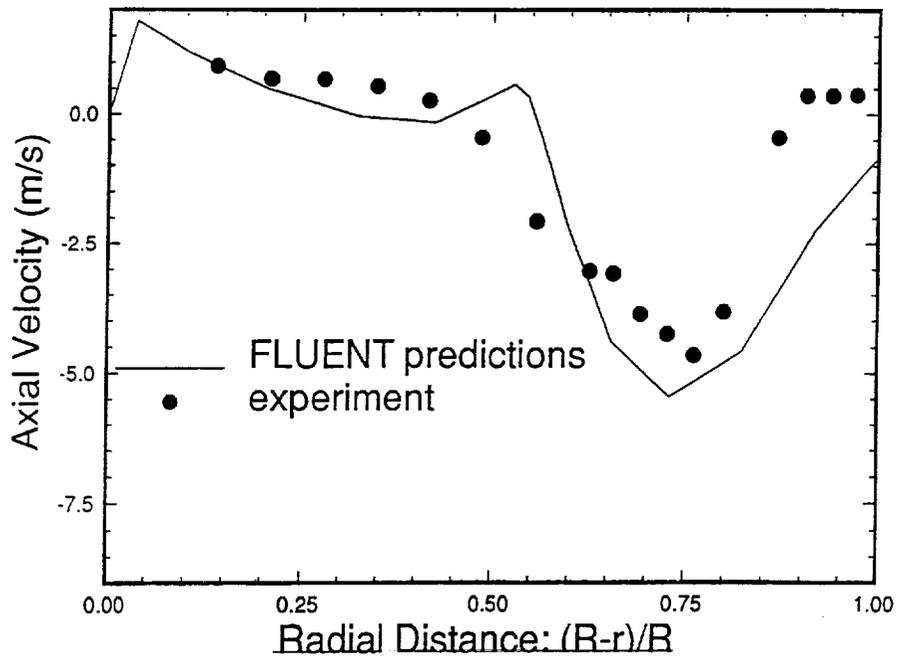
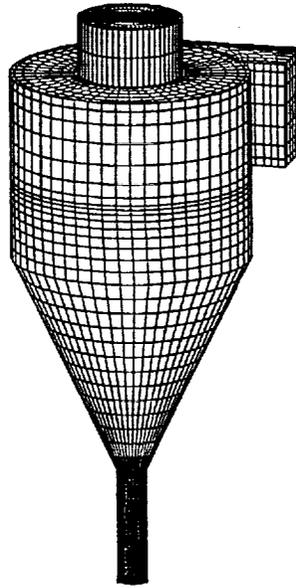
Turbulent Flow in a Transition Duct



Contours of computed streamwise velocity
(RNG-based $k-\epsilon$ model)

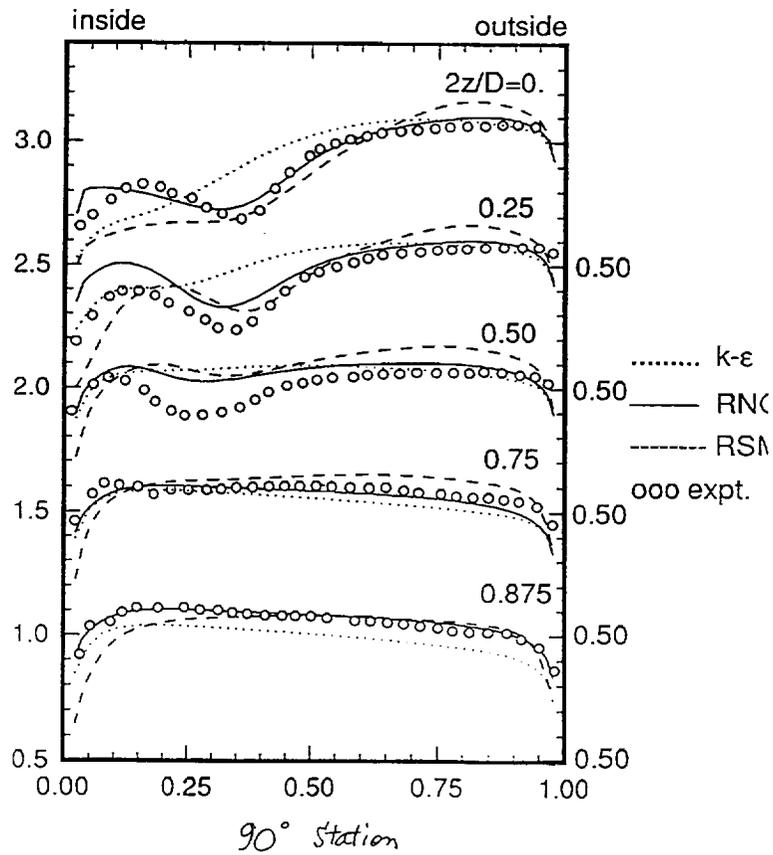
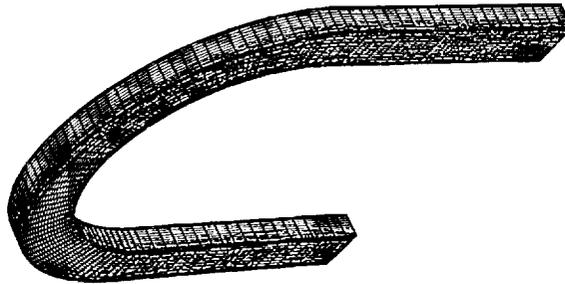
Example 2: Cyclone Sparator

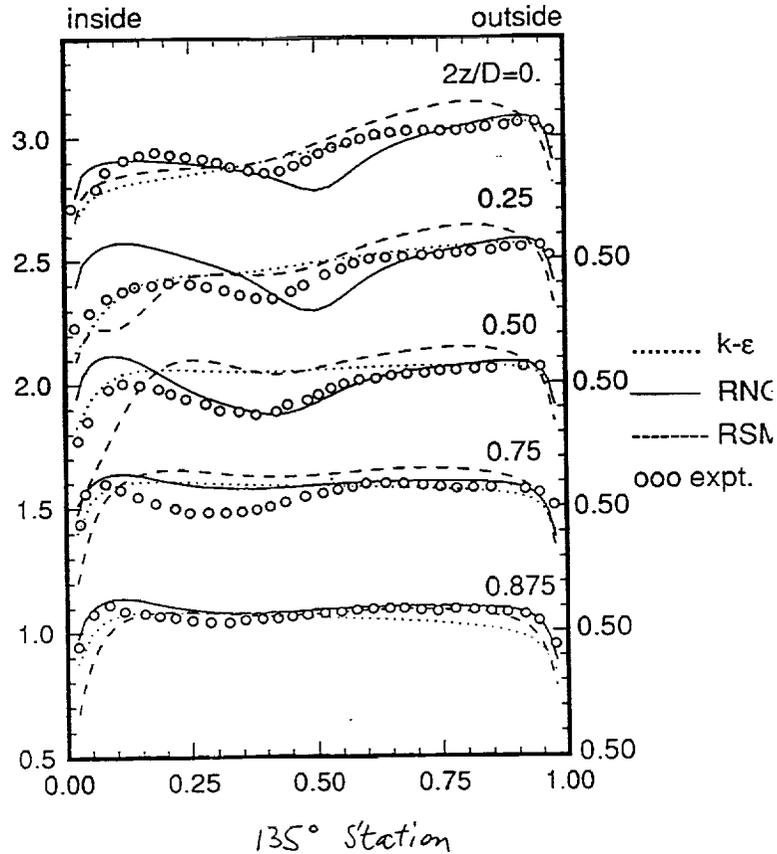
- Measured by Qing (1983).
- RSM is used.
- Cylindrical $55 \times 23 \times 41$ grid.



Example 3: 180° Bend of Square-Cross Section

- Solution Domain
 - Upstream Boundary: $5.0D_H$ from the start of the bend
 - Downstream Boundary: $5.0D_H$ from the end of the bend
 - A symmetric half of the duct modeled.
- Mesh
 - Orthogonal $101 \times 47 \times 27$
 - Distance from the wall $\approx 0.01D_H$





Part II: Combustion Modeling

- With environmental awareness, legislations on combustion-generated pollutants such as NO_x , SO_x carbon monoxide, soot, unburnt hydrocarbons, etc. have become increasingly tougher.
- Combustion simulation in industrial applications can help us to design combustors with higher efficiencies and lower pollutant emissions.
- The combustion process involves some of the most complex phenomena such as chemistry, multiphase flow, turbulence, heat transfer and the interaction between these phenomena.
- Here we focus on gaseous combustion in which the reactants may be mixed or non-mixed prior to flowing into the combustor.

Turbulence-Chemistry Interaction

- Accurate simulation of turbulent combustion requires a thorough assessment of the way turbulence and chemistry interact. The reaction rate and flame structure primarily depend on this interaction.
- In turbulent flames, chemical rates can be significantly different than those in laminar flames (sometimes several orders of magnitude), and the mean chemical rate is not the same as the rate calculated based on mean values of the various scalars:

$$\bar{r}(\theta_1, \theta_2, \dots) \neq r(\bar{\theta}_1, \bar{\theta}_2, \dots)$$

- Turbulent-chemistry interaction is best characterized by the Damkohler number which is the ratio of characteristic flow time to chemical reaction time:

$$Da = \frac{\tau_F}{\tau_r} = \frac{l}{U_f \tau_r}$$

- When $Da \ll 1$ chemical reactions are orders of magnitude slower than turbulent mixing and the influence of turbulence on reaction can be neglected.
- When $Da \gg 1$ chemical reactions are very fast and hence combustion is controlled by turbulent mixing.
- At high Da we can exploit the laminar flame concept: turbulent flame is comprised of an array of laminar flames (flamelets). Hence chemical rate expressions can be those obtained in laminar flames and the effect of turbulence can be characterized through the probability density function (pdf).
- For turbulent diffusion flame, the pdf is usually expressed in terms of a scalar which can best characterize mixing, e.g., the mixture fraction. Since the rate of reaction is much higher than the mixing rate, we can assume that the reaction system is at equilibrium. The effect of turbulence is simply felt by the fluctuations in the mixture fraction. The mean value of any scalar in the flame is simply:

$$\bar{\theta} = \int_0^1 \theta(\xi) P(\xi) d\xi$$

- For turbulent premixed flames the pdf is usually expressed in terms of a scalar which can best characterize the reaction progress, e.g., normalized temperature:

$$\bar{r} = \int_0^1 r(c) p(c) dc$$

FLUENT Equilibrium Model

- For turbulent diffusion flames we use a two-moment beta pdf and equilibrium data to calculate various thermo-chemical scalars in the flame.
- To obtain equilibrium data we use the popular CHEMKIN library of SANDIA, fully interfaced with our codes. CHEMKIN contains data on all important gaseous fuels, combustion intermediates and products as well as their properties.
- We obtain the mean mixture fraction and its variance from their respective conservation equations:

$$\frac{\partial}{\partial x_i}(\rho u_i \bar{\xi}) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{\sigma_t} \frac{\partial \bar{\xi}}{\partial x_i} \right)$$
$$\frac{\partial}{\partial x_i}(\rho u_i \overline{\xi'^2}) = \frac{\partial}{\partial x_i} \left(\frac{\mu_t}{\sigma_t} \frac{\partial \overline{\xi'^2}}{\partial x_i} \right) + \frac{2\mu_t}{\sigma_t} \left(\frac{\partial \bar{\xi}}{\partial x_i} \right)^2 - C_d \rho \frac{\mu_t}{k} \overline{\xi'^2}$$

- To save computational time we calculate the integrals before the CFD calculations.

Concluding Remarks

- As of now, we provide our users with three turbulence models:
 - the “conventional” k - ϵ model,
 - the ReNormalization Group model,
 - the Reynolds-Stress Model.
- The Renormalization group k - ϵ model has broadened the range of applicability of two-equation turbulence models.
- The Reynolds-stress model has proved useful for strongly anisotropic flows such as those encountered in cyclones, swirlers and combustors.
- Issues remain, such as near-wall closure, with all classes of models.
- Collaborative research with ICOMP will not only serve to further quantify applicability of turbulence models but may bring to market new ideas in the field of turbulence modeling for industrial flows.

OUTLINE

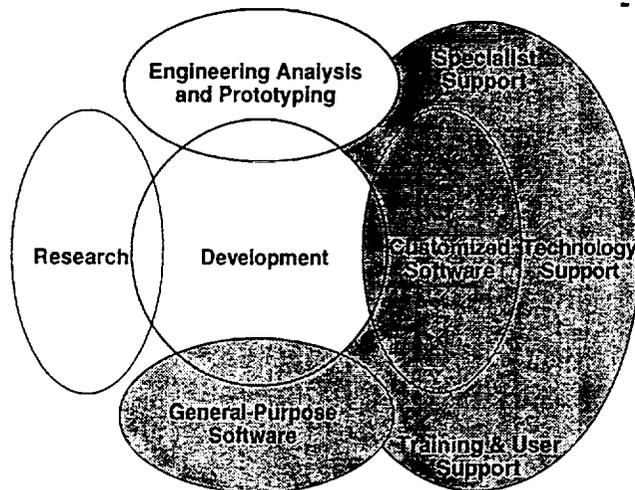
- Introduction to CFDRC
- Experiences with 2-Equation Models
 - Models Used
 - Numerical Difficulties
 - Validation and Applications
 - Strengths & Weaknesses
- Answers to Three Questions (Posed by Workshop Organizing Committee)
 1. What Are Your Customers Telling You?
 2. What Are You Doing In-House?
 3. How Can NASA-CMOTT Help?

INTRODUCTION TO CFDRC

- Young and Energetic (Turbulent) Organization, Dedicated to the Continuous Process of Advancement and Effective Transfer of CFD Technology
- TWO TYPES OF COMPLEMENTARY ACTIVITIES:

- PROJECTS

- SOFTWARE



INTRODUCTION TO CFDRC (Continued)

- **Objective User of Turbulence Models (0, 1, and 2 Equation Models, RSM and LES)**
- **Humble Developer, e.g. Monte Carlo Joint Scalar PDF**
- **Active Participant in Recent Small Eddies of Turbulence, e.g.**
 - **Stanford Endeavor: "Collaborative Testing of Turbulence Models" 1989-1993**
 - **National Workshops at: NASA MSFC, LeRC/CMOTT, etc. 1987-1994**
 - **ASME/Fluids Engineering Division, Biathlon, Lake Tahoe, June 1994**

TWO-EQUATION MODELS USED

- **Standard k- ϵ Model (Launder & Spalding, 1974)**
- **Low-Re k- ϵ Model (Chien, 1982)**
- **Extended k- ϵ Model (Chen & Kim, 1987)**
- **Multiscale k- ϵ Model (Kim & Chen, 1988)**
- **RNG-Based k- ϵ Model (Yakhot et. al. 1993)**
- **2-Layer k- ϵ Model (Rodi, 1991)**
- **k- ϵ^{++} Models**
- **k- ω Model (Wilcox, 1991)**

++ Models with Corrections for: Curvature, Rotation, Buoyancy, Compressibility, etc.

NUMERICAL DIFFICULTIES

- **Positivity of k & ε (or ω) Is Not Guaranteed in Iterative Algorithms**
- **Strong Nonlinearity of Source Terms and Coupling Causes Numerical Difficulties**
- **Inappropriate Specifications of ε (or ω) at Boundaries or in Initial Conditions May Also Cause Divergence**
- **Non-orthogonality of Grids Adds to Difficulties**
- **Non-smooth Change Over for Two-Layer Model Hinders Convergence**

VALIDATIONS PERFORMED

- **Channel and Pipe Flows**
- **Backward-Facing Step**
- **Turnaround Duct**
- **Swirl-Flow Combustor**
- **Rotating Disk Cavities**
- **Boundary Layers**
- **Jets, Wakes, and Mixing Layers**
- **Periodic Wakes Behind Bluff Bodies**

Examples of Successes and Failures

1) Flow Around a Square Cylinder; 2) 180° Square Duct; 3) S-Shaped Annular Diffuser; 4) Dump Combustor; 5) Backward Facing Step

FLOW AROUND A SQUARE CYLINDER

Strouhal Number

$$\text{Strouhal Number} = \frac{fH}{U_o}$$

f = Frequency of Vortex Shedding

H = Obstacle Height

U_o = Freestream Velocity

Model/Expt.	Time Period	Strouhal Number
Expt.	7.25	0.138
Standard k-ε	7.1	0.141
2-Layer k-ε	7.1	0.141
RNG k-ε	7.6	0.132

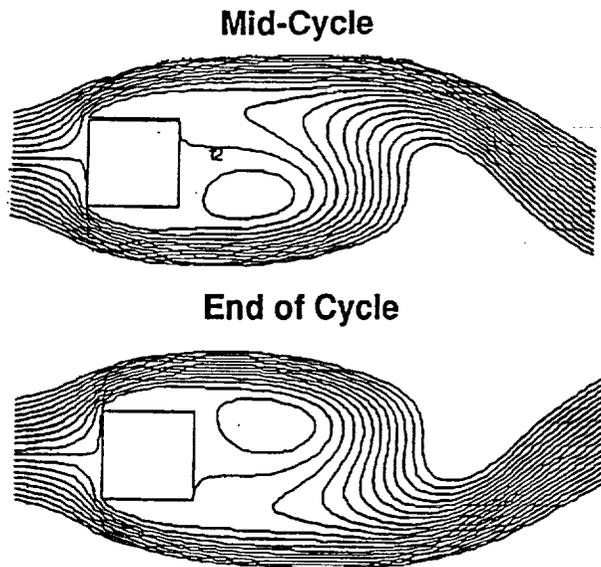
Notes:

1. Experiments By Durao, Heitor, and Pereira (1988)
2. Computations with CFD-ACE
Inlet: 78H Upstream; Outlet: 22H Downstream
Grid: 120 x 80
Time Steps: Over 70 Per Time Period

Ref.: Avva, R.K., Singhal, A.K., Lai, Y.G., "Numerical Simulation Of Periodic and 3-Dimensional, Turbulent Flows With CFD-ACE," ASME Fluid Dynamics Conference, Lake Tahoe, NV, June 19-23, 1994.

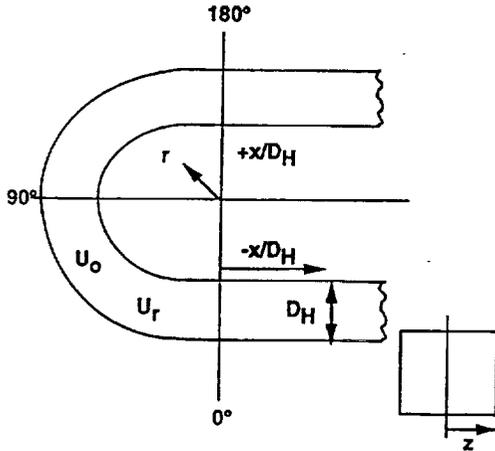
FLOW AROUND A SQUARE CYLINDER

Instantaneous Streamlines

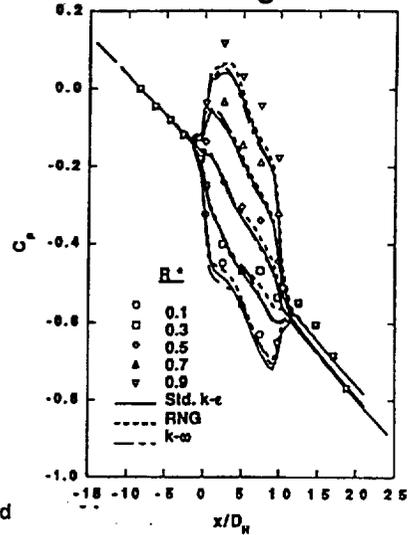


FLOW IN A 180° SQUARE DUCT

Computational Domain



Static Pressure Along Duct Walls

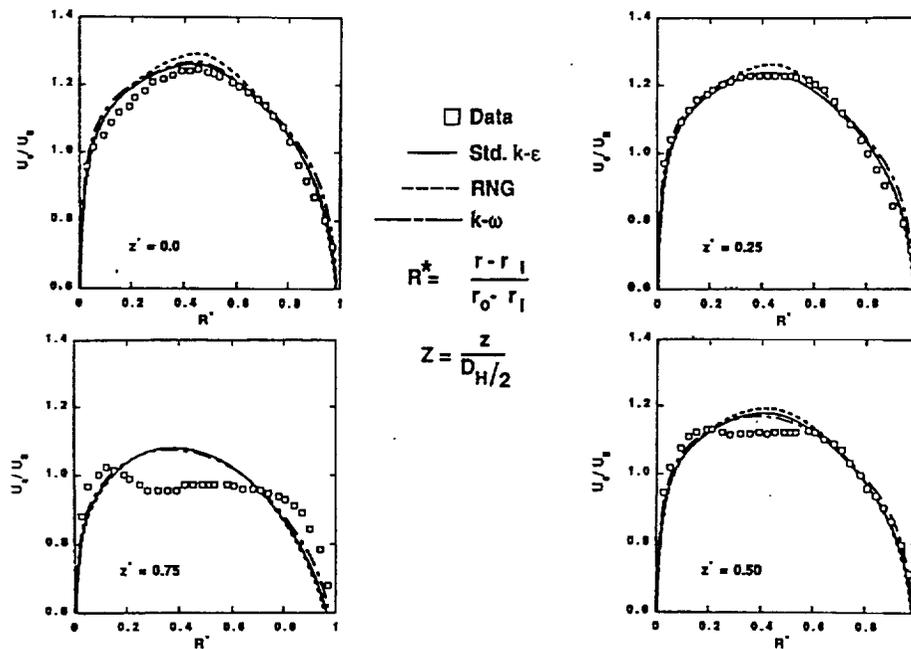


- Experiment by Chang, Humphrey and Modavi (1983)
- Computations Done with CFD-ACE on a 40x40x20 Grid

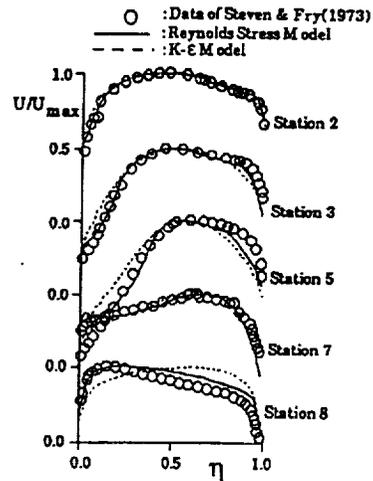
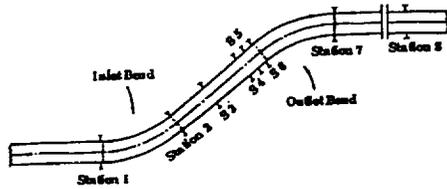
Ref.: Avva, R.K., Singhal, A.K., Lai, Y.G., "Numerical Simulation Of Periodic and 3-Dimensional, Turbulent Flows With CFD-ACE," ASME Fluid Dynamics Conference, Lake Tahoe, NV, June 19-23, 1994.

FLOW IN A 180° SQUARE DUCT

Mean Axial Velocity at $\theta = 3^\circ$

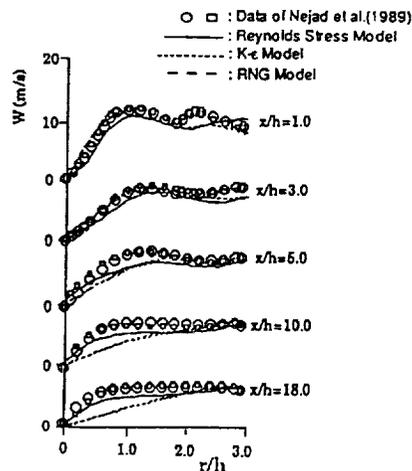
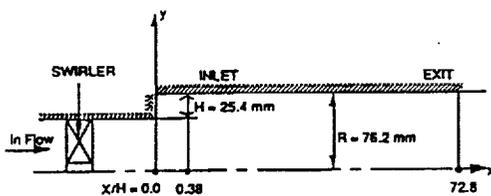


S-SHAPED ANNULAR DIFFUSER



- * k-ε Model and RNG Model Failed to Predict the Correct Location of the Maximum Velocity Downstream
- * Computations with CFD-ACE; Publication Under Preparation

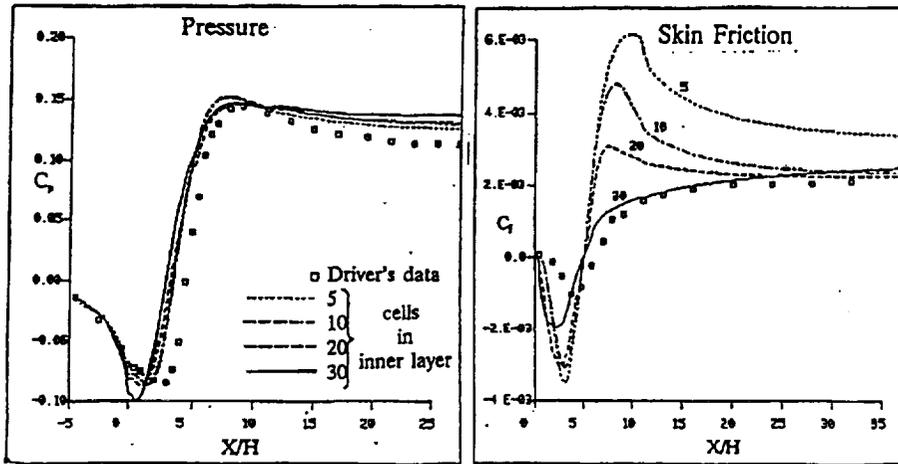
Confined Swirling Flow for a Dump Combustor



- * K-ε model failed to preserve the vortex core strength near center (see $x/h=10$ & 18)
- * Computational results to be presented at 1994 ASME Winter Annual Meeting (Chicago)

BACKWARD-FACING STEP

Sensitivity to Grid Refinement



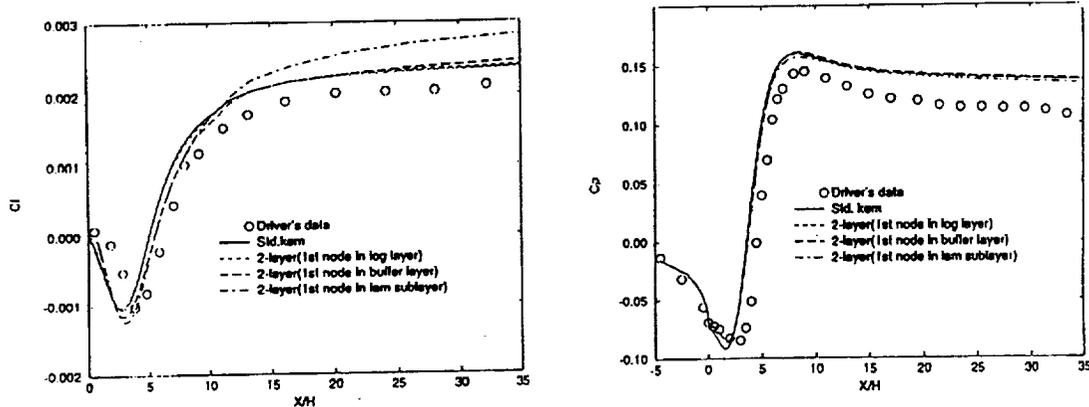
- Low-Re Model Requires >30 Nodes in the Inter Layer

Ref. : "Comparative Study of High and Low Reynolds Number Versions of k- ϵ Models," R.K. Avva, C.E. Smith, A.K. Singhal, AIAA-90-0246.

BACKWARD FACING STEP

2-Layer Model;

80 x 60 Grid, Central Differencing



Computations with CFD-ACE; To Be Published

EXAMPLE APPLICATIONS

- Gas Turbine Combustors
- Liquid Rocket Engines
- Seals and Bearing Cavities
- Impellers, Inducers, and Fans
- IC Engines
- CFD Reactors
- External Aerodynamic Flows
- Plus Many More

STRENGTHS & WEAKNESSES

Strengths of 2-Equation Models

- Numerically Economical
- Easy to Modify
- Reasonable Applicability Within Engineering Accuracy

Weaknesses

- Use of Wall Functions Requires First Grid Outside the Viscous Sublayer. This is Difficult to achieve, *a Priori*
- Low-Re Approach Does Not Offer Overall Advantage.
- Two-Layer Approach Needs More Work (e.g. Smoothing)
- Reynolds Analogy Inadequate for Heat-Transfer Applications.
- Effect of Surface Roughness on Turbulence.

CMOTT/CP QUESTIONS

- 1. What Are Your Customers Telling You?**
- 2. What Are You Doing In-House?**
- 3. How Can NASA-CMOTT Help?**

WHAT ARE CUSTOMERS TELLING?

- **PLEASE Don't Confuse Us,
with Additional Models and False Hopes**
- **Conclusions (Confusion) Over Last 15-Years**
 - **Use $k\sim\varepsilon$ Model, with Wall Functions**
 - **Wall Functions, Oh No!, Never!!
Use Low-Re $k\sim\varepsilon$,.: Which One?, How?? (Good Questions)**
 - **$k\sim\varepsilon$ Is No Good; Neglects Non-Isotropy, etc., etc.**
 - **Jump on RSM Wagon, Now!
It Can Take You Anywhere, Eventually!!**
 - **Look How Great is this $k\sim\varepsilon^{++}$
When and How to Use it? (Good Questions)**
 - **Look How Accurate is this Scheme, No Numerical Diffusion.
Don't Contaminate the Solutions with Turbulence**

WHAT IS CFDRC DOING?

- **Using What is Available, in Best Possible Ways**
- **Listening to Both Sides (Model Developers and Users)**
- **Trying to Resist Peer Pressures**
- **Struggling to Find Resources for Mundane Goals Such as Developing Guidelines for Correct Use of Turbulence Models**

HOW CAN CMOTT HELP?

- **CMOTT Has Been Providing Commendable Service in the Very Difficult Subject: Turbulence**
- **"Turbulence Subprogram" Should Help Further**
- **Additional Effort is Needed in Many Areas, Such As:**
 - **Near Wall Treatment**
 - **Effect of Surface Roughness**
 - **Economical Heat Transfer Model**
 - **Documentation of Experiences in:**
 - a) **Model Robustness(In Addition to Accuracy)**
 - b) **Model Sensitivity to Grid Distribution and Boundary Conditions**
 - **Transition Model (if Possible Suitable for $k-\epsilon$ Framework)**

HOW CAN CMOTT HELP? (Continued)

- **NASA-CMOTT Is One of the Few Groups Sustaining Momentum for Turbulence Modeling.**
- **It Is In Unique (Privileged) Position for Embracing the Challenge of Developing Specific Recommendations (Guidelines) For:**
 - a) **Selection of Adequate Models for Different Class of Problems**
 - b) **Correct Use of Each Model**
- **The Task Is Difficult But Practical**
- **Select Fewer Roads, Post Milestones, and Go Further**
- **Move An Inch Closer to Users**





PROGRESS IN SIMULATING INDUSTRIAL FLOWS USING TWO-EQUATION MODELS:
CAN MORE BE ACHIEVED WITH FURTHER RESEARCH?

N95-27895

Vahé Haroutunian
Fluid Dynamics International, Inc.
Evanston, Illinois

BACKGROUND AND OBJECTIVES

- ▶ Two-equation eddy-viscosity models (TEM's) are the most cost effective for the purposes of applied CFD. Give best accuracy vs. cost balance.
- ▶ There is a lot of confusion about true strengths and limitations of TEM's especially that of standard k - ϵ model.
- ▶ We have embarked on extensive study of TEM's over wide range of flows:
 - ▷ Identify true strengths and limitations of standard k - ϵ model.
 - ▷ Evaluate other TEM's.
 - ▷ Assess emerging models and novel modeling trends.
 - ▷ Identify key areas requiring further research.
- ▶ This talk provides brief review of TEM's from perspective of applied CFD.
 - ▷ It provides objective assessment of both well-known and newer models.
 - ▷ It compares model predictions from various TEM's with experiments.
 - ▷ It identifies sources of modeling error and gives historical perspective of their effects on model performance and assessment.
 - ▷ It recommends directions for future research on TEM's.

REMARK:

- ▶ Many reported poor predictions of TEM's are primarily due to combination of improper choice of near-wall model and over-diffuse numerics.
- ▶ TEM performance can be much improved from further research in:
 - ▷ Length scale determining equation.
 - ▷ Advanced (Anisotropic/Nonlinear) Eddy-viscosity models.

INTRODUCTION AND BACKGROUND

○ About FDI

- ▶ Over 10 years in business.
- ▶ Primary product FIDAP (FluId Dynamics Analysis Package).

○ About FIDAP

- ▶ First commercial general-purpose finite element CFD program.
- ▶ Models wide range of flows.
- ▶ Over 700 FIDAP licenses worldwide.

○ FIDAP Turbulence Modeling Capabilities

- ▶ Based on two-equation eddy-viscosity models:
 - ▷ Standard k - ϵ model (Launder and Spalding).
 - ▷ Extended k - ϵ model (Chen and Kim).
 - ▷ RNG k - ϵ model (Yakhot, Orszag, Thangam, Gatski and Speziale).
- ▶ Low-Re near-wall modeling based on two-layer approach:
 - ▷ Viscous sublayers spanned by single layer of specialized elements.
 - ▷ van Driest's model used in viscous sublayers.
 - ▷ Interpolation functions based on universal flow profiles.
- ▶ Latest turbulence modeling enhancements (to appear soon):
 - ▷ Anisotropic eddy-viscosity models.
 - ▷ Wilcox's k - ω model.
 - ▷ Anisotropic version of the standard k - ϵ model.

○ Typical Industrial User

- ▶ Design engineer.
- ▶ Trained in fluid mechanics and heat/mass transfer.
- ▶ Familiar with range of flows of interest to his/her organization.
- ▶ NOT CFD expert.
- ▶ Little or no background in turbulence modeling.

○ Turbulence Modeling Requirements of Applied CFD Codes

- ▶ Optimal balance of cost and accuracy:
 - ▷ Turbulence modeling overhead of critical concern.
 - ▷ Overall accuracy of $\pm 15\%$ adequate for most cases.
- ▶ Consistent performance over wide range of flows:
 - ▷ Heat/mass transfer
 - ▷ 2-D and 3-D (Cartesian, axisymmetric)
 - ▷ Complex geometries
 - ▷ Transient flows
- ▶ Adaptable to a wide range of complex flow physics:
 - ▷ Low-Re effects
 - ▷ Variable density/compressibility effects
 - ▷ Combustion
 - ▷ Two-phase
- ▶ Minimum level of user input/intervention:
 - ▷ No fine tuning model coefficients and/or solution parameters.
 - ▷ No physical input other than boundary and/or initial conditions.
- ▶ No geometry dependence:
 - ▷ Distance to wall and/or y^+ dependence.
- ▶ Stable numerical characteristics.

TURBULENCE MODELING CONSIDERATIONS

○ Key Modeling Issues

- 1- Accurate modeling of mechanisms governing $\overline{\rho u_i' u_j'}$, $\overline{\rho u_i' \theta'}$, $\overline{\rho u_i' c_a'}$.
 - a) Pressure-scrambling
 - b) Body forces
 - c) Transport effects
 - d) Dissipation
- 2- Accurate modeling of characteristic turbulent length scales.
- 3- Accurate modeling of low-Re near-wall phenomena.

○ Optimal Level of Turbulence Model for Applied CFD

- ▶ **Second-Moment Closures (DSMC's) and (ASMC's)**
 - (+) DSMC's ideally suited to modeling aspects 1-a,b,c above, however,
 - (-) DSMC's costly, especially in 3-D in presence of heat/mass transfer.
 - (-) Geometry dependence in current pressure-scrambling models.
 - (-) ASMC's perform erratically (1-c above not well modeled).
 - (-) ASMC's numerically less stable (stiff equations).
- ▶ **Two-Equation Eddy-Viscosity/Diffusivity Models (TEM's)**
 - (+) Least costly.
 - (+) No geometry dependence (except some low-Re TEM's).
 - (+) Numerically more stable.
 - (-) Conventional TEM's not suitable for modeling effects 1-a,1-b,&1-c.
 - (+) Room for significant improvement in predicting effects of complex strain and anisotropy through the combined use of improved length scale equations and advanced eddy-viscosity models.
 - (-) Transport effects (1-c), however, cannot be directly predicted.

LENGTH SCALE DETERMINING EQUATION

○ THE STANDARD k - ϵ MODEL

$$\rho \frac{D\epsilon}{Dt} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + c_1 \frac{\epsilon}{k} G - c_2 \rho \frac{\epsilon^2}{k}$$

where,

$$G = -\overline{\rho u_i' u_j'} \frac{\partial u_i}{\partial x_j} \approx \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j}$$

and,

$$c_\mu = 0.09, \quad c_1 = 1.44, \quad c_2 = 1.92, \quad \sigma_k = 1.0, \quad \sigma_\epsilon = 1.3$$

▶ Remarks on standard k - ϵ model:

- ▶ Use is made of Boussinesq's "isotropic" viscosity model.
- ▶ Fine scale isotropy is assumed in modeling ϵ equation.
- ▶ Is high-Re model. Must be used with suitable near-wall sub-model.
- ▶ Many reported poor predictions are due to improper choice of near-wall model, mesh density, discretization scheme and boundary conditions.
- ▶ Model predicts much better than commonly believed, if used properly.
- ▶ It does however have its shortcomings in predicting difficult flows involving strong anisotropy and/or non-equilibrium effects - it tends to be over-diffuse. It predicts flatter flow profiles, shorter recirculating zones, and occasionally does not predict subtle separation bubbles.

LENGTH SCALE DETERMINING EQUATION

○ THE EXTENDED k - ϵ MODEL OF CHEN AND KIM

- ▶ Employs modified ϵ equation containing extra generation term.
- ▶ Rationale is that in addition to turbulence time scale k/ϵ , there is further time scale $\rho k/G$ characterizing response of ϵ to mean strain.

$$\rho \frac{D\epsilon}{Dt} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + c_1 \frac{\epsilon}{k} G + c_3 \frac{G^2}{\rho k} - c_2 \rho \frac{\epsilon^2}{k}$$

$$c_\mu = 0.09, c_1 = 1.15, c_2 = 1.9, c_3 = 0.25, \sigma_k = 0.75, \sigma_\epsilon = 1.15$$

▶ Remarks on extended k - ϵ model of Chen and Kim:

- ▶ Is high-Re turbulence model. Needs near-wall model.
- ▶ Gives similar predictions to standard model in equilibrium flows.
- ▶ We find Chen and Kim's (1987) recommended model produce predictions that are too under-diffuse in confined flows.
- ▶ We have tuned constants $c_1 = 1.35$ and $c_2 = 0.05$ to improve performance
- ▶ Revised model gives better results for some well-known benchmark flows, but improved predictions over standard model are not realized consistently. More experience and possibly fine tuning is needed.

LENGTH SCALE DETERMINING EQUATION

○ THE RNG k - ϵ MODEL

- ▶ RNG k - ϵ model has undergone two major revisions.
- ▶ Latest version due to Yakhot, Orszag, Thangam, Gatski, and Speziale

$$\rho \frac{D\epsilon}{Dt} = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + c_1 \frac{\epsilon}{k} G - R - c_2 \rho \frac{\epsilon^2}{k}$$

where

$$R = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u'_k}{\partial x_i} \frac{\partial u'_k}{\partial x_j} = \frac{c_\mu \eta^3 (1 - \eta/\eta_0) \epsilon^2}{1 + \beta \eta^3} k$$

$$\eta \equiv s \frac{k}{\epsilon}; \quad s = \sqrt{G/\mu_t}$$

and

$$c_\mu = 0.085, c_1 = 1.42, c_2 = 1.68, \sigma_k = \sigma_\epsilon = 0.7179, \eta_0 = 4.38, \beta = 0.015$$

- ▶ Above version is high-Re turbulence model. Needs near-wall model.
- ▶ Most testing of model has been done with simple near-wall model.
- ▶ Our testing of model with more accurate near-wall model indicates that RNG model is often under-diffusive in internal flows and can be very over-diffusive in some external flows.
- ▶ We have tuned model constants and obtained better overall predictions.
 $c_\mu = 0.0865, c_1 = 1.45, c_2 = 1.83, \sigma_k = 0.8, \sigma_\epsilon = 1.15, \eta_0 = 4.618, \beta = 0.17$
- ▶ Revised model gives better results for some well-known benchmark flows, but improved predictions over standard model are not realized consistently. More experience and possibly fine tuning is needed.

LENGTH SCALE DETERMINING EQUATION

○ Additional Remarks on RNG k - ϵ Model:

- ▶ Interesting development though no major breakthrough.
- ▶ Most model constants are predicted from RNG theory.
- ▶ In applying RNG theory it is assumed that turbulence field has very wide spectrum and that inertial sub-range is isotropic.
- ▶ Values of model constants predicted by RNG theory are approximate owing to simplifying assumptions made in applying RNG method.
- ▶ Model predictions critically dependent on additional term R .
- ▶ The R term reflects proposed contributions from fine scale anisotropy.
- ▶ The R term is not derived and modeled using RNG theory.
- ▶ The R term has essential similarities with extra term in ϵ eq'n of extended k - ϵ model of Chen and Kim.
- ▶ Latest model does not predict von Karman constant.

- ▶ **The most notable fact about the RNG k - ϵ model of YOTGS is that it challenges the notion of fine scale isotropy of turbulence**
 - ▷ Thus ϵ (and consequently the characteristic turbulent length scale) is assumed to be significantly influenced by the fine scale structure. These effects are heuristically modeled via the time scale ratio η .
 - ▷ It is interesting to note that the assumption of fine scale anisotropy used in modeling R conflicts with notion of a wide and isotropic turbulent spectrum used in applying RNG theory to rest of model.
 - ▷ It is more likely that the turbulent length scale is influenced strongly by **large scale anisotropy** as characterized by the anisotropy tensor a_{ij} .
 - ▷ Anisotropic eddy-viscosity models can provide estimates of a_{ij} which can be used to design improved length scale determining eqn's.

ADVANCED EDDY-VISCOSITY MODELS (Beyond Boussinesq)

○ Anisotropic Eddy Viscosity Models (AEVM's)

- ▶ There has been renewed emphasis in developing AEVM's.
- ▶ Lead to better approximations of the normal and shear stresses and therefore turbulence anisotropy effects.
- ▶ In addition to more accurate modeling of $\overline{\rho u_i u_j}$, AEVM's could potentially be used to improve modeling of:
 - ▷ Length scale determining eq'n.
 - ▷ Generation rate of turbulence energy.
- ▶ Examples of AEVM's are:
 - ▷ Lumely (1970)
 - ▷ Speziale (1987)
 - ▷ Yoshizawa (1984), DIA
 - ▷ Rubinstein and Baron (1990), RNG
 - ▷ Taulbee (1992) and Speziale (1993), derived from DSMC's
 - ▷ Launder (1993)

- ▶ **Remarks:**
 - ▷ Potential of models have been demonstrated using simple tests.
 - ▷ Improvements in accuracy often of second-order in magnitude.
 - ▷ Not been extensively tested especially for swirling flows.
 - ▷ Anisotropic models not yet extended to turbulent heat/mass fluxes.
 - ▷ We are presently investigating AEVM's of Speziale (1987) and Launder (1993).

THE LOW-RE NEAR-WALL MODEL

○ Wall Function Models

- ▶ Produce over-diffuse solutions in off-equilibrium boundary layers.
 - ▷ Often fail to predict separation or vortex shedding.
- ▶ Unfortunately still in extensive use in applied CFD codes.

○ Specialized Finite Element Model (FIDAP)

- ▶ Is essentially two-layer model.
- ▶ Avoids fine near-wall mesh via use of one layer of specialized elements.
- ▶ Employs van Driest's low-Re mixing-length model in near-wall layer.
- ▶ Combines low cost of wall function models with accuracy of two-layer models.
- ▶ y^+ dependence confined to single layer and transparent to user.

Remarks:

- ▶ Most of historical testing and verification of TEM's has been done using wall functions. The excess diffusion has lead to much confusion in assessing TEM's.
- ▶ Proper assessment of TEM's requires at least two-layer models.
- ▶ Wall function approach is simply unacceptable for applied CFD.

IMPACT OF DISCRETIZATION ERROR

○ Sources of Discretization Error:

- ▶ Grid refinement (grid convergence).
- ▶ Location of computational boundaries (e.g., outlet, inlet, entrainment).
- ▶ Choice of discretization scheme in space and time.

Remarks:

- ▶ Effect of discretization error has received less attention in turbulence model development and testing.
- ▶ Most serious source of error results from discretization of advection terms (i.e., the *upwinding scheme*).
- ▶ Common but dangerous upwinding strategy is used in many CFD codes:
 - ▷ Use accurate unbounded scheme in mean flow equations.
 - ▷ Use inaccurate numerically diffuse scheme in turbulence equations.
 - ▷ Overall scheme is stable but often highly diffusive.
 - ▷ Most of development and testing of turbulence models has been done using above upwinding strategy.
 - ▷ In our computations we employ the accurate **streamline upwind (SU)** scheme in both mean and turbulence equations.
 - ▷ Even more accurate schemes are available which are based on Petrov-Galerkin finite element formulations.
- ▶ Accurate schemes must be used in both mean flow and turbulence eq's.

NUMERICAL RESULTS

- Free Jets
 - ▶ Round jet
 - ▶ Plane jet
- Internal Flows with Separation
 - ▶ Flow past backward facing step (Kim et. al)
 - ▶ Flow past step in channel with diffuser wall (Driver and Seegmiller)
 - ▶ Flow in pipe expansion (Szzepura)
- Transient Flow (Vortex Shedding)
 - ▶ Flow past square prism (Lyn)
- 3-D Flow
 - ▶ Flow past passenger car models

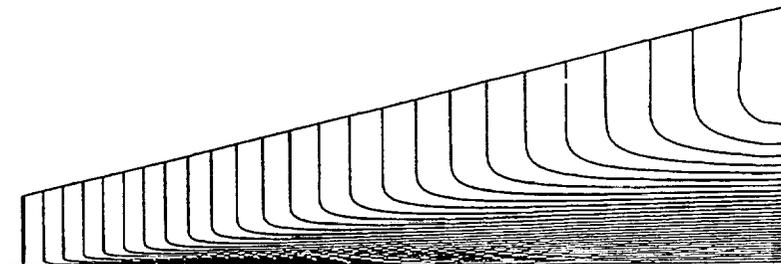
REMARKS:

- ▶ Five sets of model predictions are presented:
 - ▷ Standard $k-\epsilon$ model
 - ▷ Extended $k-\epsilon$ model (original)
 - ▷ Extended $k-\epsilon$ model (revised)
 - ▷ RNG $k-\epsilon$ model with (original)
 - ▷ RNG $k-\epsilon$ model with (revised)

FREE JETS

The Submerged Plane and Round Jets

	Plane Jet		Round Jet	
	$d\delta/dx$	% error	$d\delta/dx$	% error
Experiment	=0.105		=0.095	
Standard $k-\epsilon$ model	0.104	-1	0.112	18
Extended $k-\epsilon$ model (original)	0.10	-5	0.10	5
Extended $k-\epsilon$ model (revised)	0.102	-3	0.104	9.5
RNG $k-\epsilon$ model (original)	0.131	25	0.157	65
RNG $k-\epsilon$ model (revised)	0.101	-4	0.113	19



TURBULENT FLOW OVER BACKWARD FACING STEP

Kim et al Test Case: $Re = 45000$

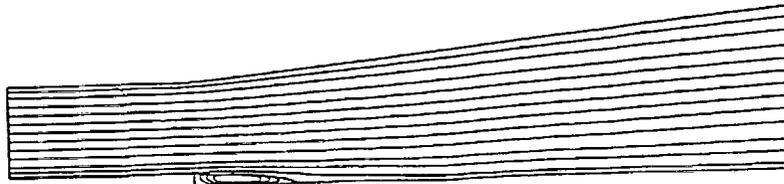
	X_R	% error
Experiment	7.0 ± 0.5	
Standard $k-\epsilon$ model	6.5	-7.1
Extended $k-\epsilon$ model (original)	8.4	20.0
Extended $k-\epsilon$ model (revised)	7.1	1.4
RNG $k-\epsilon$ model (original)	7.5	7.1
RNG $k-\epsilon$ model (revised)	7.46	6.6



TURBULENT FLOW OVER STEP IN CHANNEL WITH
DIFFUSER WALL

Driver and Seegmiller Test Case: $Re = 36000$

	Angle			
	0 degrees		6 degrees	
	X_R	% error	X_R	% error
Experiment	6.2		8.1	
Standard $k-\epsilon$ model	5.3	-14.5	6.6	-18.5
Extended $k-\epsilon$ model (original)	6.6	6.5	9.55	17.9
Extended $k-\epsilon$ model (revised)	5.76	-7.1	7.4	-8.6
RNG $k-\epsilon$ model (original)	6.17	-0.5	8.33	2.8
RNG $k-\epsilon$ model (revised)	6.11	-1.5	8.33	2.8



TURBULENT FLOW IN PIPE EXPANSION

Szczepura Test Case: $Re = 890,000$

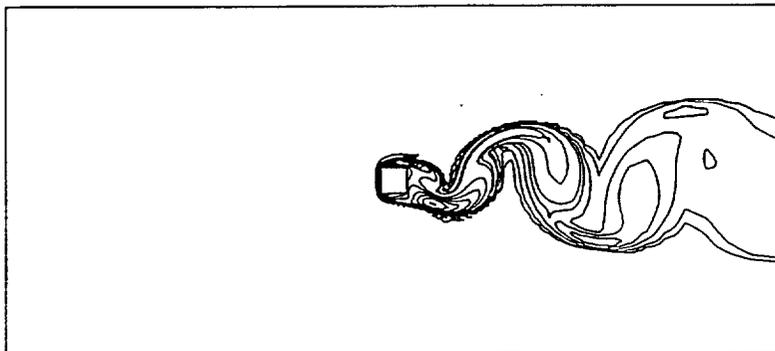
	X_R	% error
Experiment	9.51	
Standard $k-\epsilon$ model	9.59	0.9
Extended $k-\epsilon$ model (original)	12.44	30.8
Extended $k-\epsilon$ model (revised)	10.6	11.5
RNG $k-\epsilon$ model (original)	11.35	19.5
RNG $k-\epsilon$ model (revised)	11.39	20



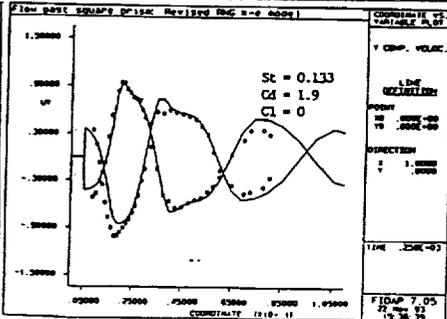
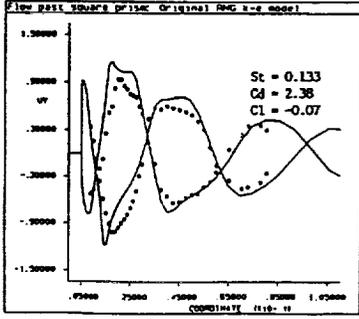
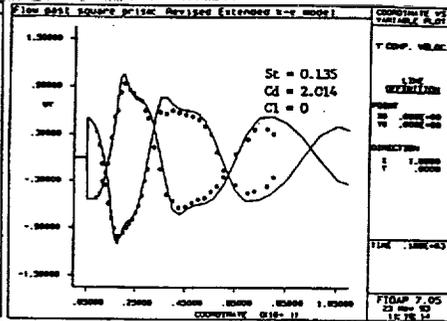
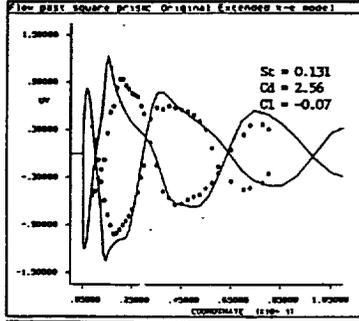
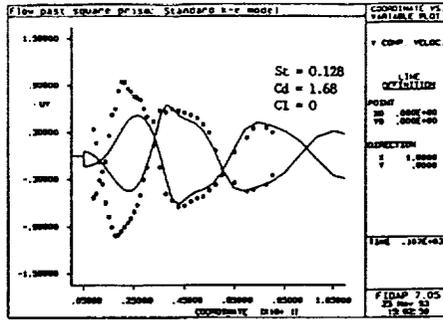
TURBULENT FLOW PAST SQUARE PRISM

Lyn's Test Case: $Re = 21400$

	Strouhal No.	C_d	C_l
Experiment	0.132 ± 0.035	≈ 2.0	N.A.
Standard $k-\epsilon$ model	0.128	1.68	0
Extended $k-\epsilon$ model (original)	0.131	2.56	-0.07
Extended $k-\epsilon$ model (revised)	0.135	2.014	0
RNG $k-\epsilon$ model (original)	0.133	2.38	-0.07
RNG $k-\epsilon$ model (revised)	0.133	1.9	0

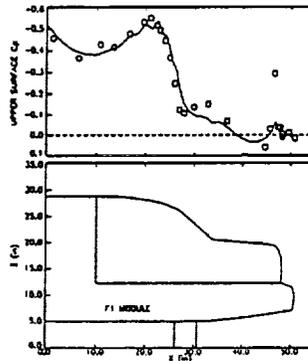
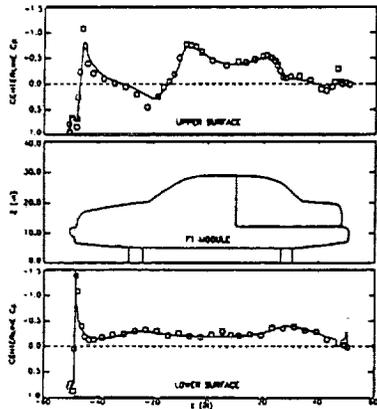


Experimental Data
 $St = 0.132 \pm 0.035$
 $Cd = 2.0$
 $Cl = \dots$

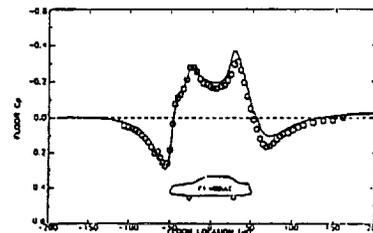
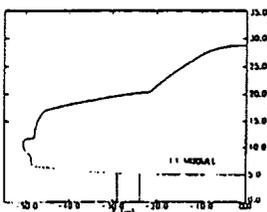
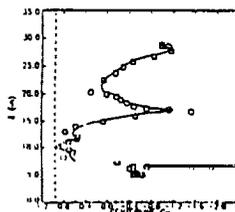


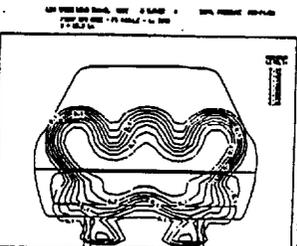
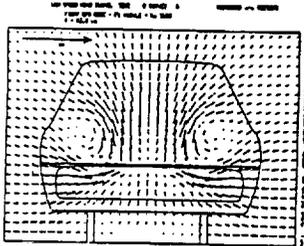
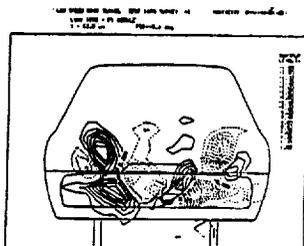
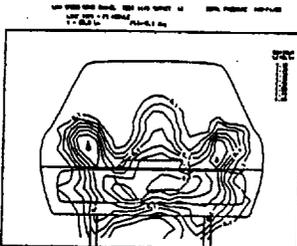
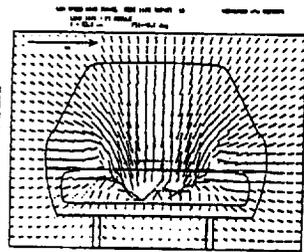
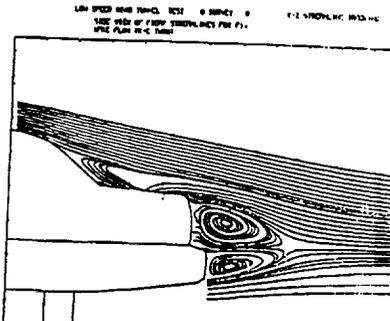
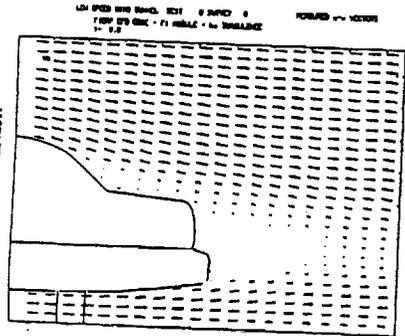
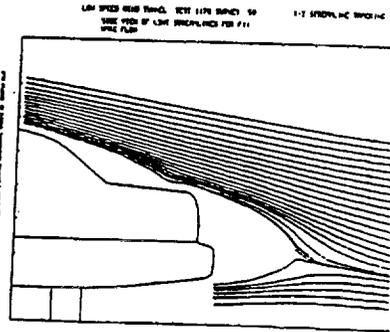
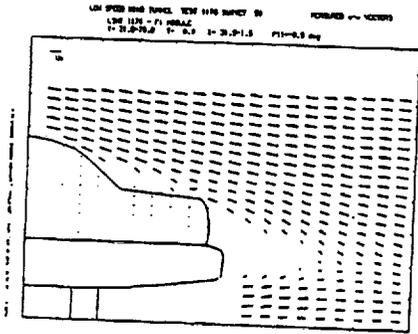
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 — FIDAP CFD CODE - ke TURB



DRAG COEFFICIENT
 Experiment .1808
 Prediction .1897

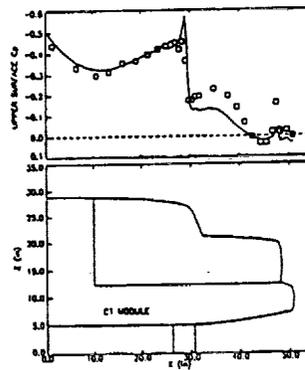
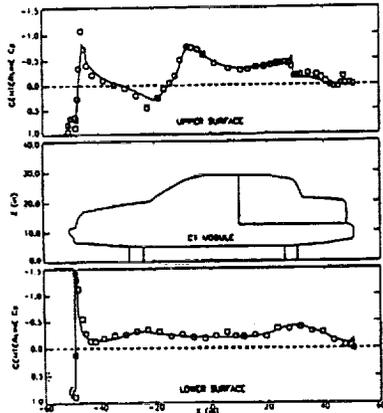




LOW SPEED WIND TUNNEL

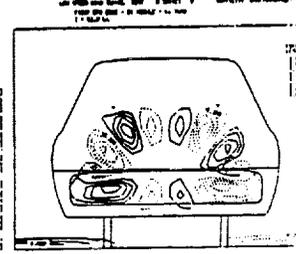
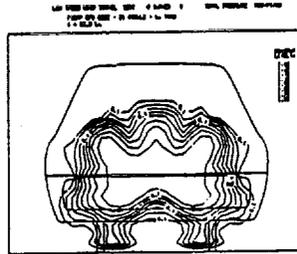
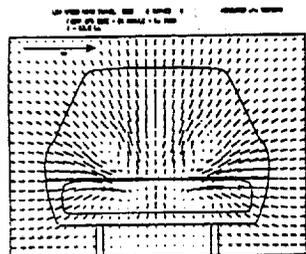
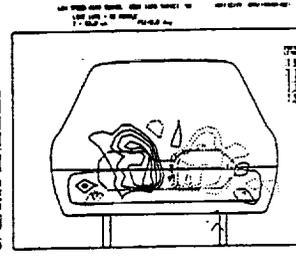
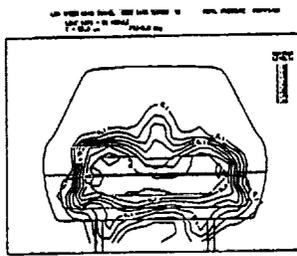
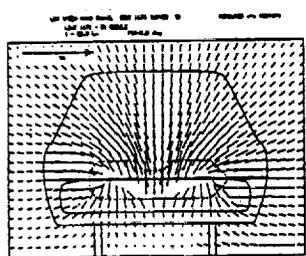
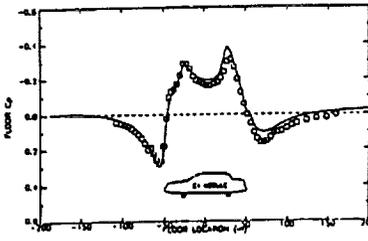
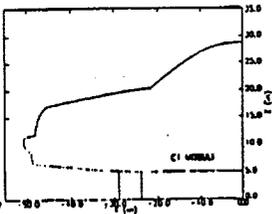
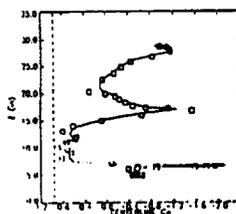
Cp DATA

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 — FIDAP CFD CODE - Mc TURB

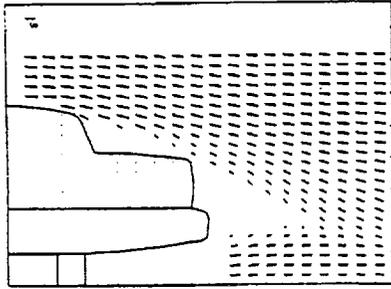


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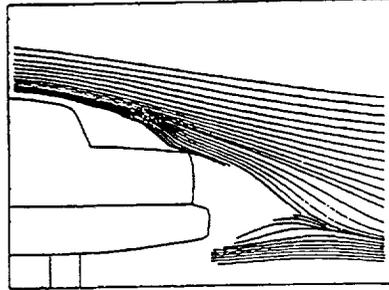
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 Prediction .1697



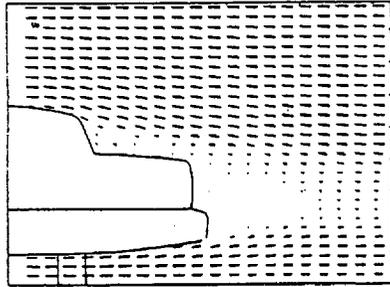
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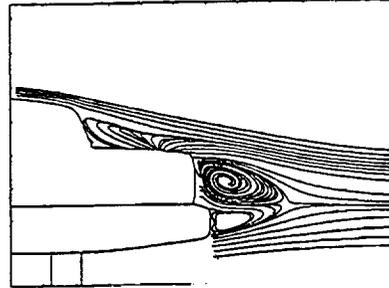
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 CASE 1118 - ST. MIDDLE
 11-21-87-10.8 11-21-87-1.3 11-21-87-1.3



LOW SPEED WIND TUNNEL TEST 1176 IMPACT OF
 CASE 1118 - ST. MIDDLE - 1/4 TURN
 11-21-87-10.8

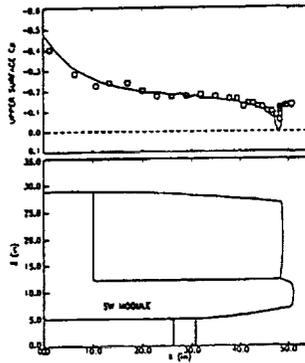
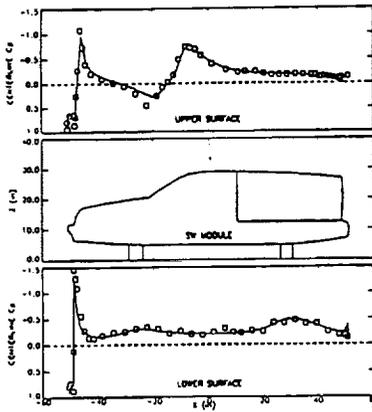


LOW SPEED WIND TUNNEL TEST 1176 IMPACT OF
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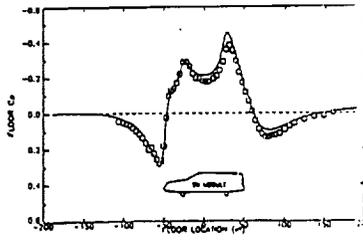
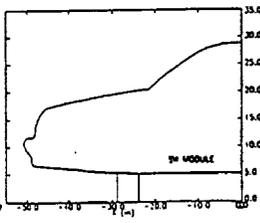
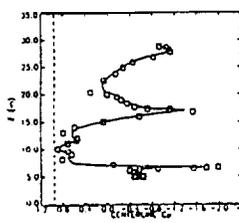


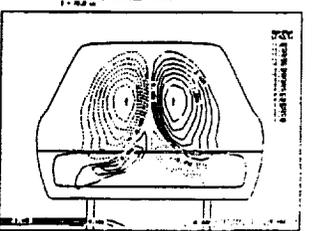
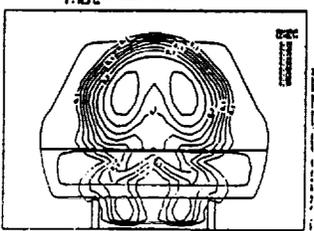
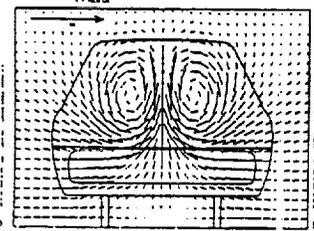
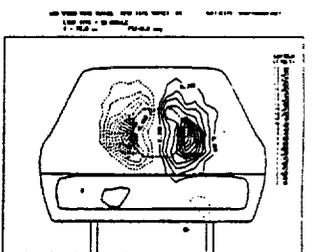
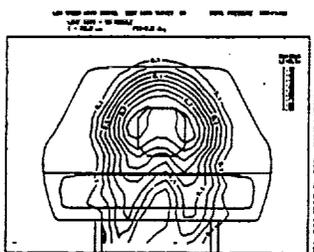
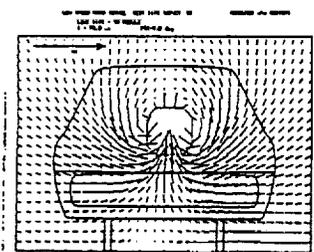
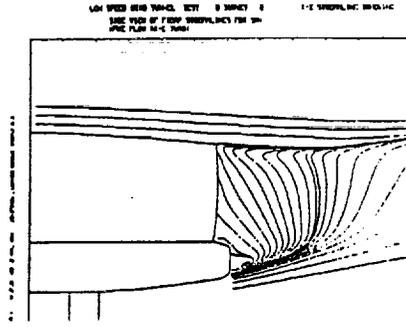
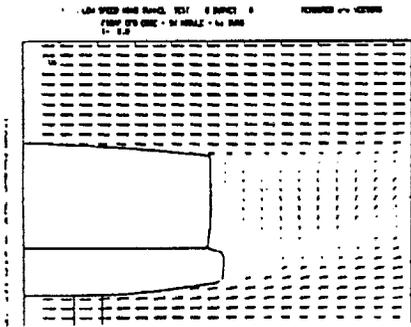
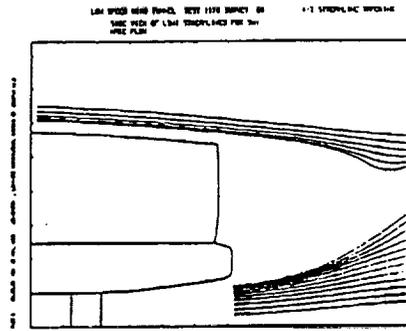
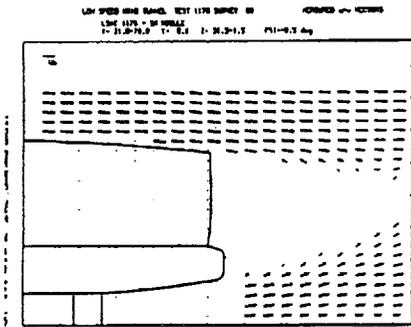
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□ LSWT 1176 RUN 10 PT 13
 — FIDAP CFD CODE - no TURB



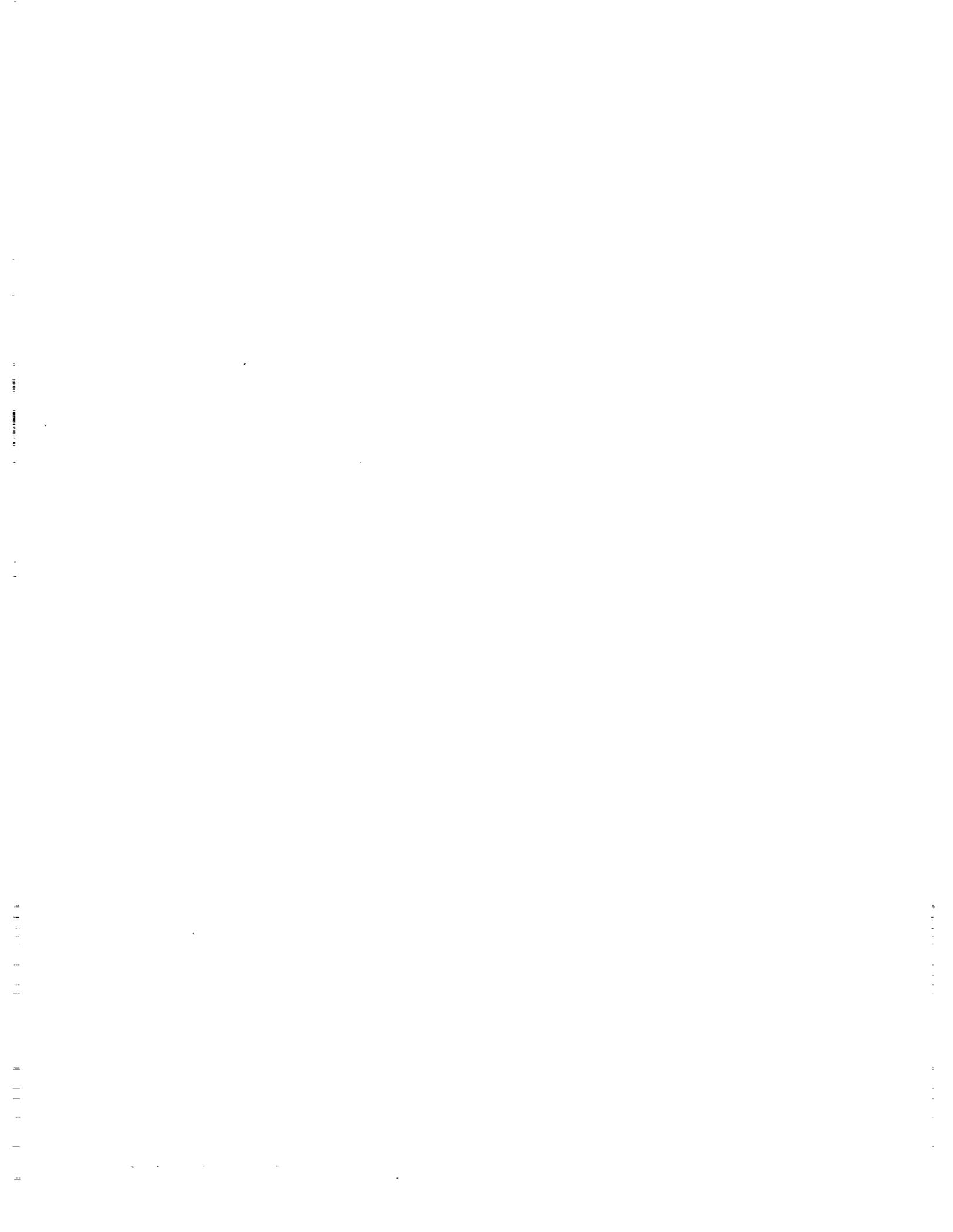
DRAG COEFFICIENT
 Experiment .1996
 Prediction .2289





CONCLUSIONS AND DIRECTIONS FOR FURTHER RESEARCH

- ▶ For applied CFD, TEM's strike balance between accuracy and efficiency.
- ▶ The use of inadequate near-wall models and over-diffuse numerical schemes obscures true performance characteristics of TEM's. And this has lead to much confusion in evaluation of TEM's.
- ▶ Consequences of using better near-wall model and accurate numerics are:
 - ▷ Standard k - ϵ model performs much better than commonly believed.
 - ▷ Extended k - ϵ model with original set of model constants produces under-diffuse predictions.
 - ▷ RNG k - ϵ model with original set of model constants gives predictions that can be both under-diffusive or over-diffusive depending on flow.
 - ▷ The extended and RNG models with revised set of model constants perform better than with original set of model constants.
- ▶ Newer models are quite promising, but do not yet perform consistently better than standard k - ϵ model.
- ▶ Significant advances in TEM capabilities may potentially result from further research in two key areas:
 - ▷ Advanced constitutive-type laws for the Reynolds stresses:
 - AEVM's appear to be best candidates.
 - ▷ Improved length scale determining equation:
 - Better modeling of off-equilibrium effects.
 - Better modeling of large-scale anisotropy effects.



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CONTENT OF PRESENTATION

- **STAR-CD: COMPUTATIONAL FEATURES**
- **STAR-CD: TURBULENCE MODELS**
- **COMMON FEATURES OF INDUSTRIAL COMPLEX FLOWS**
- **INDUSTRY-SPECIFIC CFD DEVELOPMENT REQUIREMENTS**
- **INDUSTRIAL COMPLEX FLOWS: APPLICATIONS & EXPERIENCES**
 - **FLOW IN ROTATING DISC CAVITIES**
 - **DIFFUSION HOLE FILM COOLING**
 - **INTERNAL BLADE COOLING**
 - **EXTERNAL CAR AERODYNAMICS**
- **CONCLUSION: TURBULENCE MODELING NEEDS**

STAR-CD: COMPUTATIONAL FEATURES

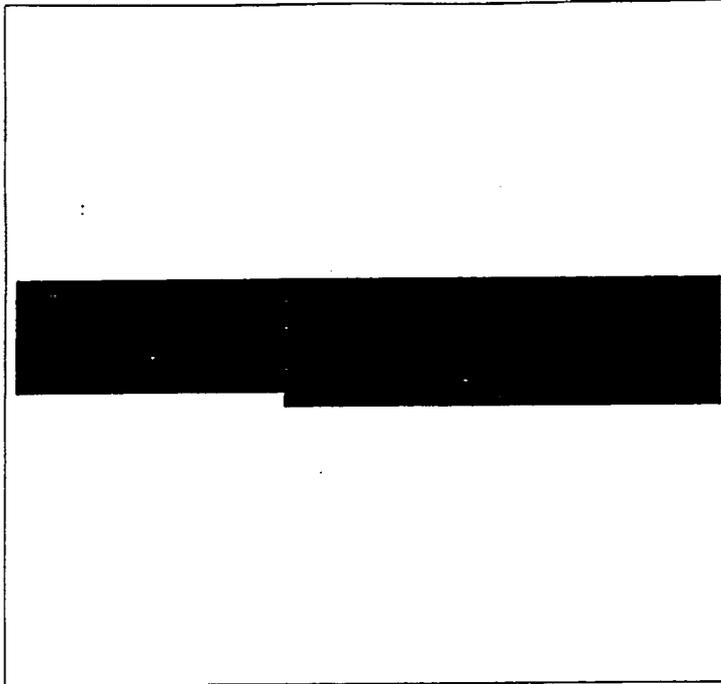
- **BODY-FITTED NON-ORTHOGONAL COORDINATE SYSTEM**
- **UNSTRUCTURED COMPUTATIONAL MESH, DIFFERENT CELL TOPOLOGIES, IMBEDDED MESH REFINEMENT, DISCONTINUOUS MESH INTERFACE, MOVING BOUNDARY AND INTERNAL INTERFACES**
- **PRIMITIVE VARIABLE, SELF-ADAPTIVE ELLIPTIC-HYPERBOLIC PRESSURE CORRECTION METHOD**
- **COLLOCATED-VARIABLE ARRANGEMENT**
- **EULER-IMPLICIT TEMPORAL INTEGRATION**
- **UD, CD, LUD, SFCD SPATIAL DISCRETIZATION, WITH BLENDING CAPABILITY**

STAR-CD: TURBULENCE MODELS

- TWO-EQUATION MODEL
 - STANDARD $k-\epsilon$ WITH CORRECTIONS FOR BULK DILATATION AND BUOYANCY
 - HIGH REYNOLDS NO. RNG BASED $k-\epsilon$ MODEL
- TWO-ZONE (TWO-LAYER) MODEL
 - HIGH REYNOLDS NO.: $k-\epsilon$ VARIANTS
 - LOW REYNOLDS NO.: $k-\epsilon$ VARIANTS, PRANDTL MIXING LENGTH MODEL

STAR-CD: TURBULENCE MODELS

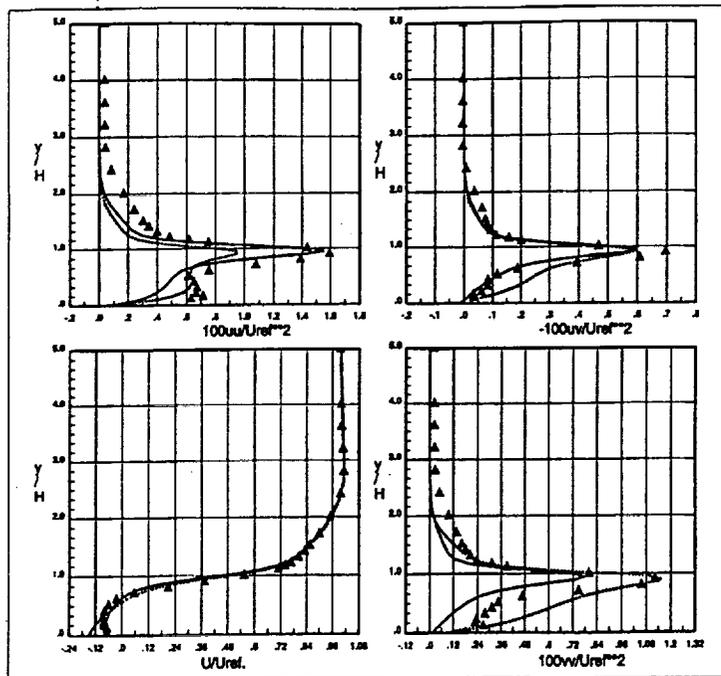
- REYNOLDS STRESS TRANSPORT MODEL
 - TRANSPORT EQUATIONS FOR CARTESIAN STRESS TENSOR IN NON-ORTHOGONAL COORDINATE SYSTEM, ON NON-STRUCTURED MESH
 - LAUNDER, RODI, REECE (1975) FORMULATION WITH LAUNDER (1989) MODEL CONSTANTS
 - GIBSON & LAUNDER (1978) WALL REFLECTION MODEL



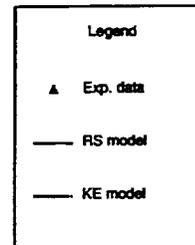
Sep 94
 VIEW
 .000
 .000
 1.000
 ANGLE
 .000
 DISTANCE
 .340
 CENTER
 .076
 .057
 .003
 EHIDDEN PLOT



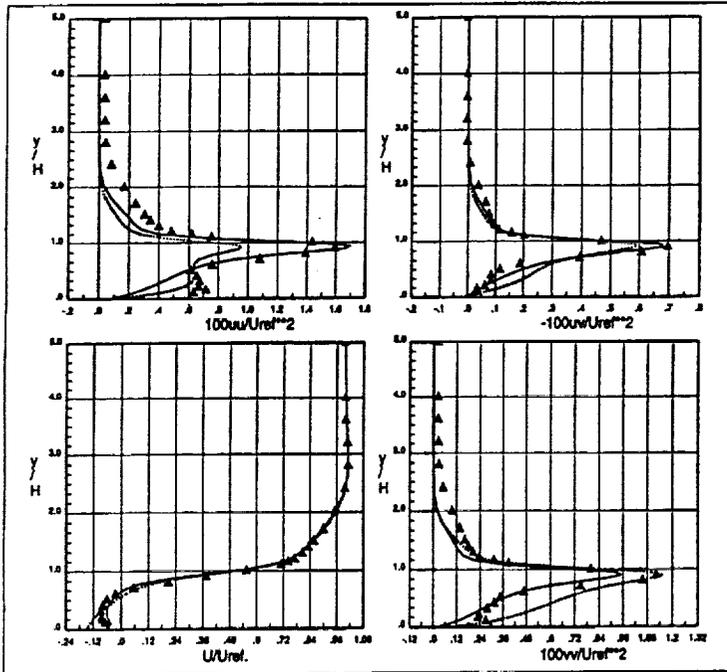
Driver & Seegmiller Backward Facing Step
 Flow Domain = -20*H to 32*H
 Mesh = 105 (Axial) x 45 (Radial)



GRAPH PLOT
 FRAMES

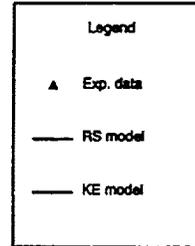


Driver & Seegmiller Backward Facing Step
 Data Inlet B.C.
 Location X/H = 1.5

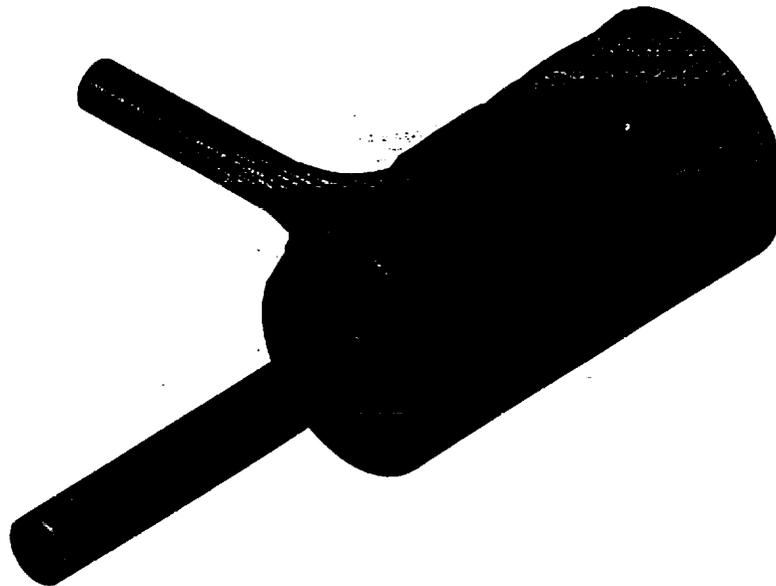


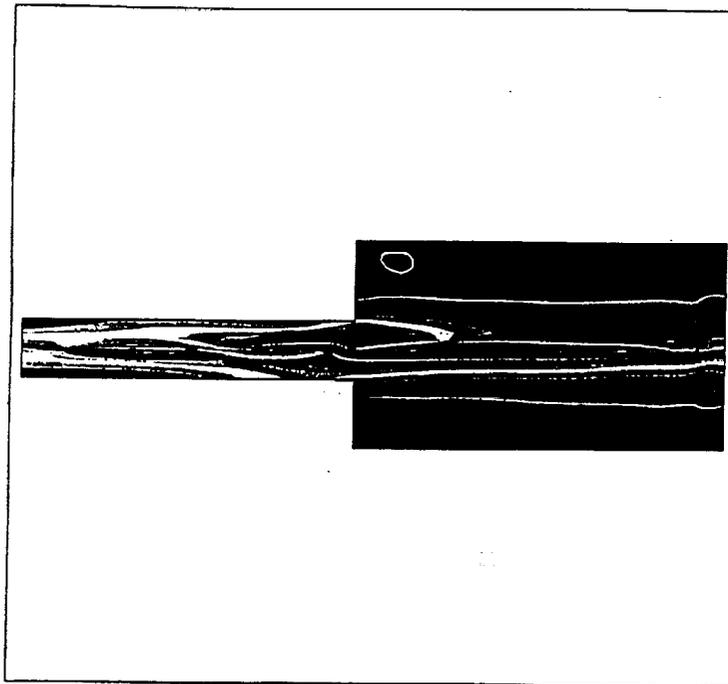
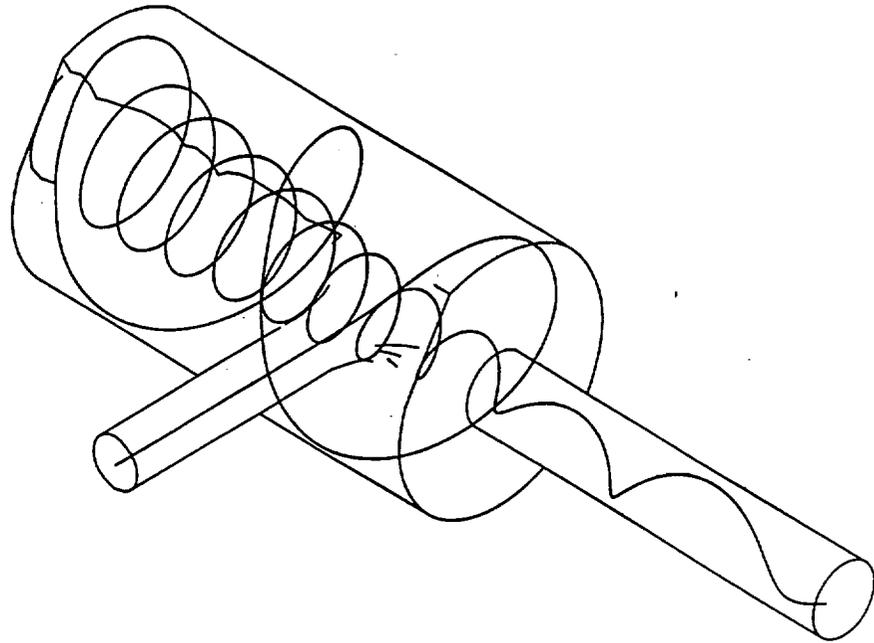
7 Sep 84

GRAPH PLOT
FRAMES

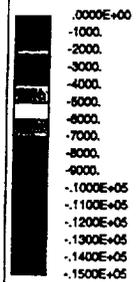


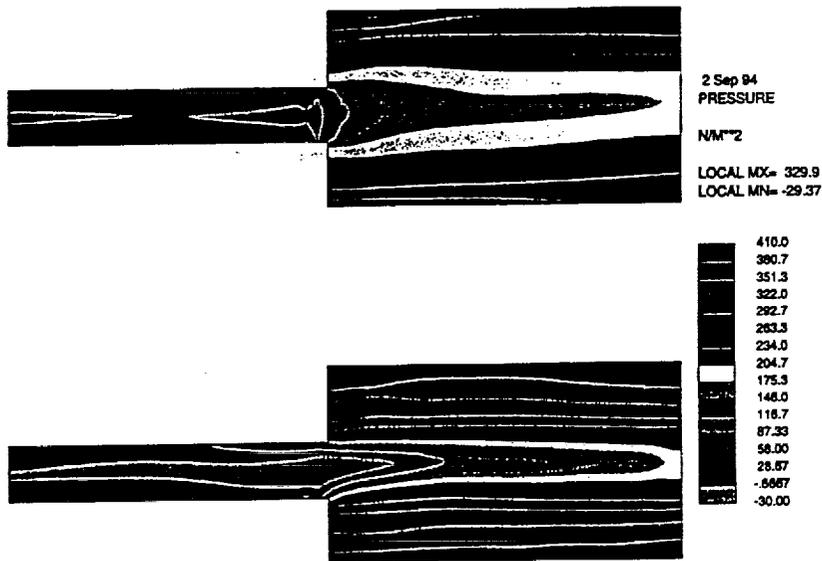
Driver & Seegmiller Backward Facing Step
Data Inlet B.C.; No Wall Damping Funct.
Location $X/H = 1.5$





8 Sep 94
ROTATIONAL SPEED
RPM
PSYS=99
LOCAL MX= .4226E+05
LOCAL MN= -.8288E+05





0.5 LUD DIFFERENCING
TURBULENCE MODEL KE - UPPER, RSM - LOWER

COMMON FEATURES OF INDUSTRIAL COMPLEX FLOWS

- **THREE DIMENSIONAL WITH MULTIPLE FLOW "COMPLEXITIES"**
 - BODY-FORCE FIELDS
 - STREAM SURFACE CURVATURE
 - STRONG PRESSURE GRADIENTS
 - COMPRESSIBILITY EFFECTS
 - LAMINAR-TURBULENT TRANSITION
 - COMBUSTION, SHOCK, MULTIPHASE, NON-NEWTONIAN
- **LARGE SCALE DOMAIN AND COMPLEX GEOMETRIC CONFIGURATION**
- **IRREGULAR, UNSTRUCTURED COMPUTATIONAL MESH**
- **SPATIAL RESOLUTION DIFFICULT TO ACHIEVE ON $O(10^5 - 10^6)$ MESH CELLS**
- **INSUFFICIENT AND UNCERTAIN EXPERIMENTAL DATA FOR TURBULENCE MODEL VALIDATION/IDENTIFICATION OF DEFICIENCIES**

INDUSTRY-SPECIFIC CFD DEVELOPMENT REQUIREMENTS

- **AUTOMOTIVE INDUSTRY**

- EFFICIENT COMPLEX-GEOMETRY, MOVING-BOUNDARY CAPABILITIES
- MEMORY/SOLUTION PERFORMANCE FOR LARGE SCALE DOMAIN CFD SIMULATION
- DIAGNOSTIC/COMPARATIVE EVALUATION OBJECTIVES
- GEOMETRIC FIDELITY AND SPATIAL RESOLUTION ARE PRIMARY ACCURACY FACTORS

- **AEROSPACE INDUSTRY**

- REGULAR AND SMALL-SCALE FLOW DOMAIN (BENCHMARK EXPERIMENTAL MODELS)
- DESIGN/PERFORMANCE OPTIMIZATION OBJECTIVES
- NUMERICAL AND TURBULENCE MODEL ACCURACY IMPORTANT
- REQUIREMENTS
 - HEAT TRANSFER
 - LOW REYNOLDS NO. FLOW
 - BODY FORCE FIELDS

ORIGINAL PAGE IS
OF POOR QUALITY

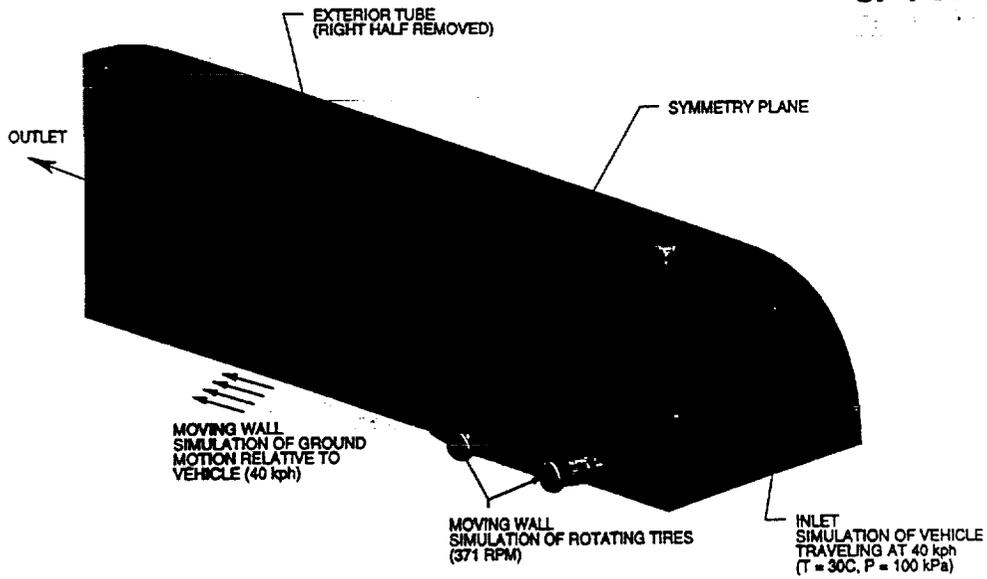
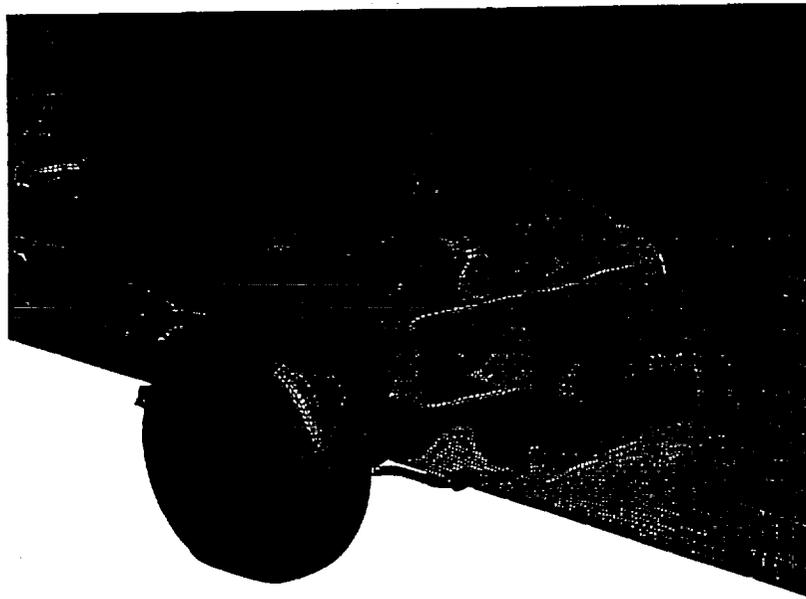
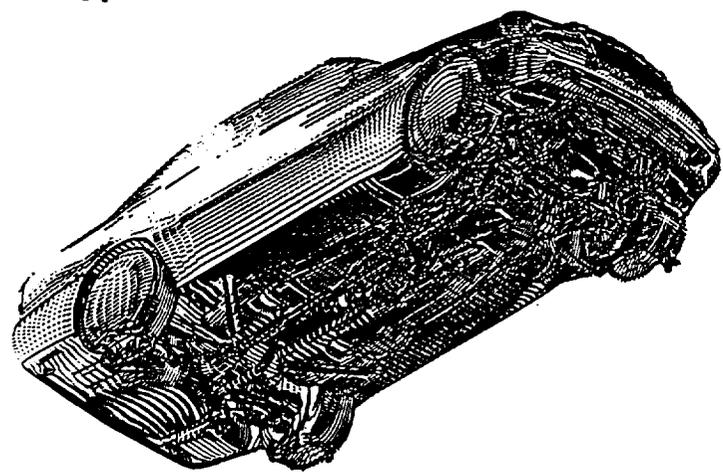


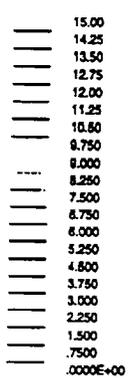
FIGURE 1: EXTERIOR BOUNDARY CONDITIONS FOR W202 40 kph ANALYSIS



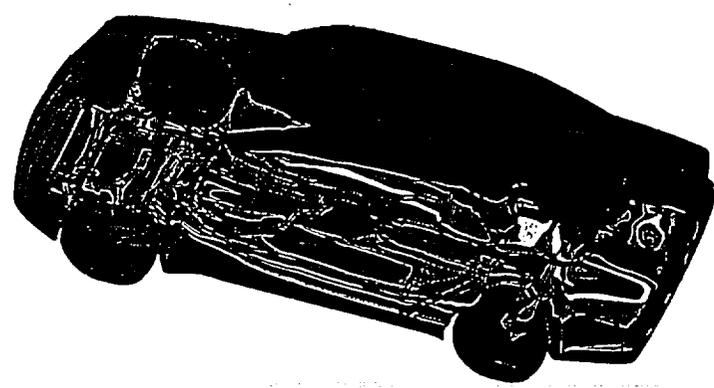
ORIGINAL PAGE IS
OF POOR QUALITY



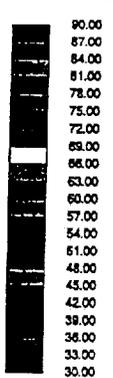
11 Dec 93
VELOCITY MAGNITUDE
M/S
ITER = 140
LOCAL MX = 50.81
LOCAL MN = .0000E+00



W202 UNDERHOOD FLOW ANALYSIS
CASE 3: 40 kph SIMULATION
Velocity near the surface of the vehicle.



9 Dec 93
TEMPERATURE
Degrees C
LOCAL MX = 210.9
LOCAL MN = .0000E+00



W202 UNDERHOOD FLOW ANALYSIS
CASE 3: 40 kph SIMULATION

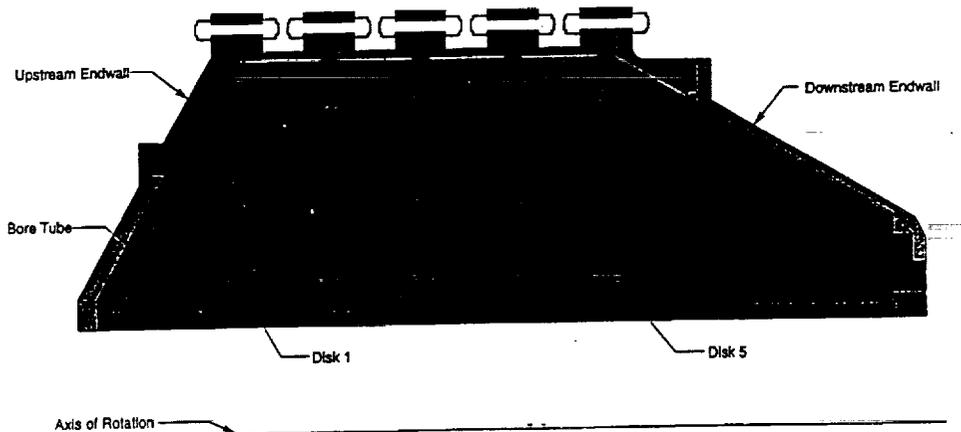
APPLICATIONS & EXPERIENCES

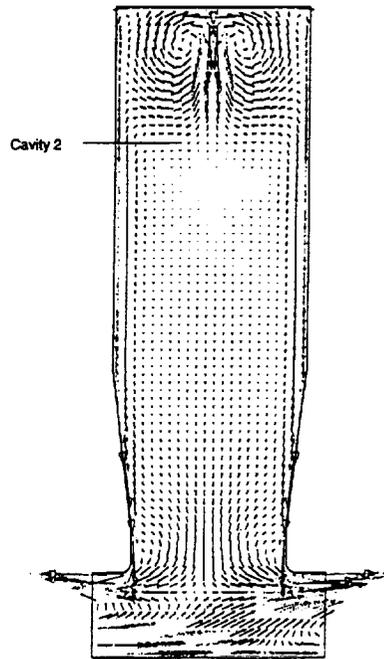
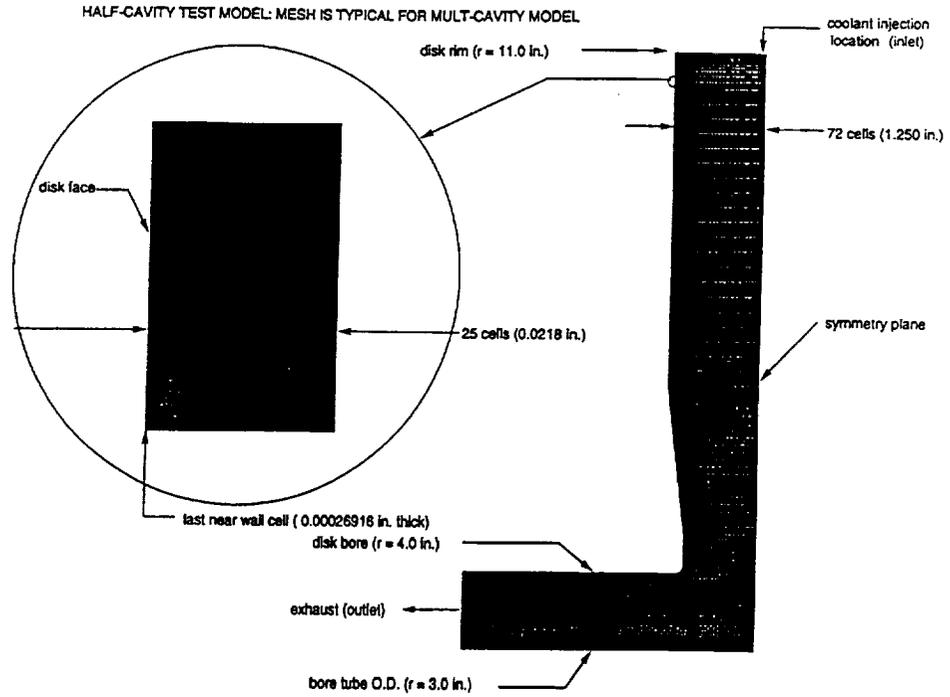
APPLICATION (DATA)	FLOW COMPLEXITY	TURBULENCE MODEL	FINDINGS	T.M. NEEDS
ROTATING DISC CAVITY ¹	<ul style="list-style-type: none"> • FORCE FIELD • WALL EFFECT 	<ul style="list-style-type: none"> • $k-\epsilon$ • 2 LAYER $k-\ell$ 	<ul style="list-style-type: none"> • EKMAN LAYER RESOLVED • FAIR PRESSURE DROP • EXCESSIVE E.V. 	<ul style="list-style-type: none"> • RSTM + SUITABLE 2 LAYER • LOW Re RSTM
DIFFUSION HOLE FILM COOLING ²	<ul style="list-style-type: none"> • JET-CROSS FLOW • WALL ANISOTROPY 	<ul style="list-style-type: none"> • $k-\epsilon$ • RNG, $k-\epsilon$ • 2 LAYER $k-\ell$ 	<ul style="list-style-type: none"> • JET SEPARATION SENSITIVE TO MESH TOPOLOGY/ RESOLUTION • POOR SPANWISE SPREAD 	<ul style="list-style-type: none"> • RSTM + SUITABLE 2 LAYER • LOW Re RSTM

¹ GRABER et al (1987)

² GOLDSTEIN et al (1968), LIGRANI et al (1992)

COMPRESSOR DRUM TEST RIG STAR-CD CONJUGATE HEAT TRANSFER MODEL

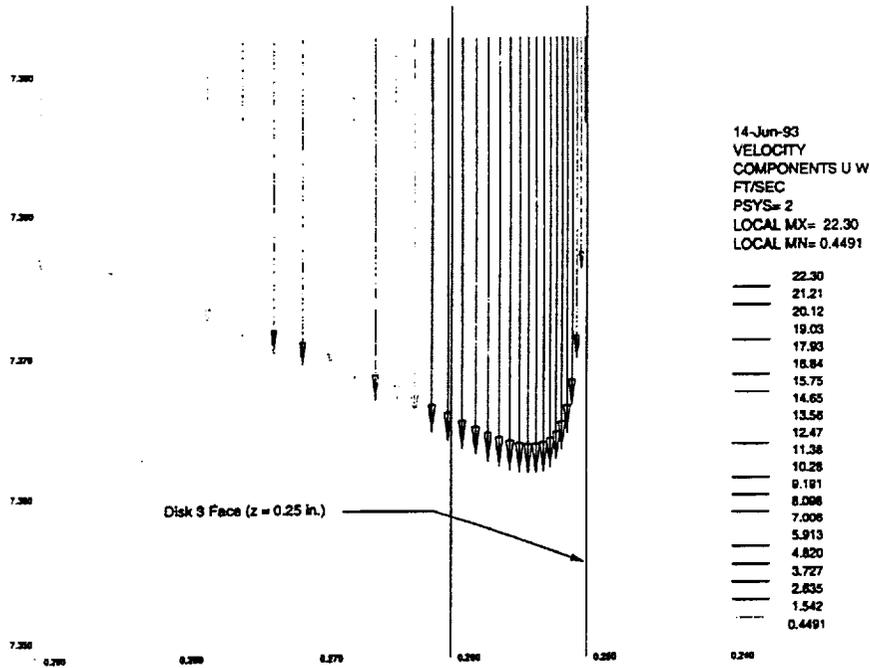




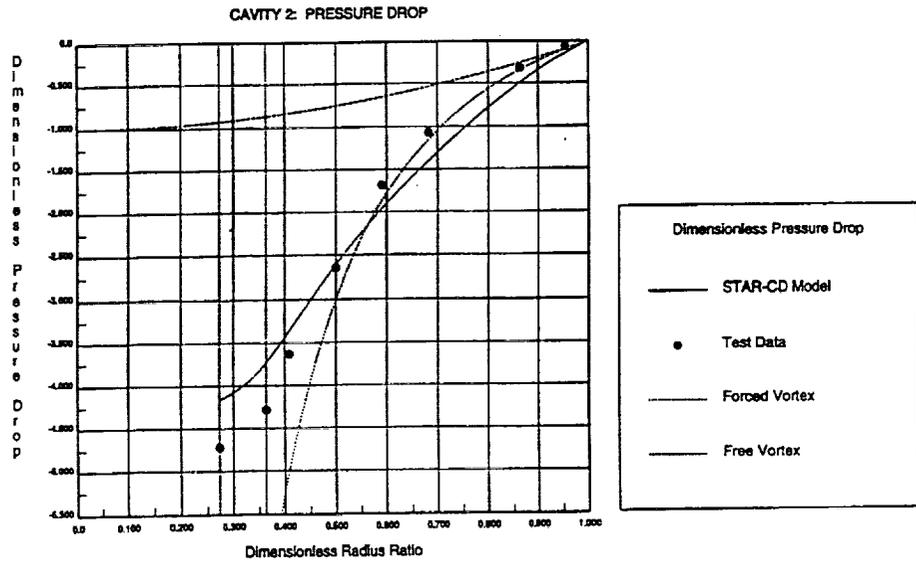
14-Jun-93
 VELOCITY
 COMPONENTS U W
 FT/SEC
 PSYS= 2
 LOCAL MX= 36.44
 LOCAL MN= 0.2792E-01
 PRESENTATION GRID

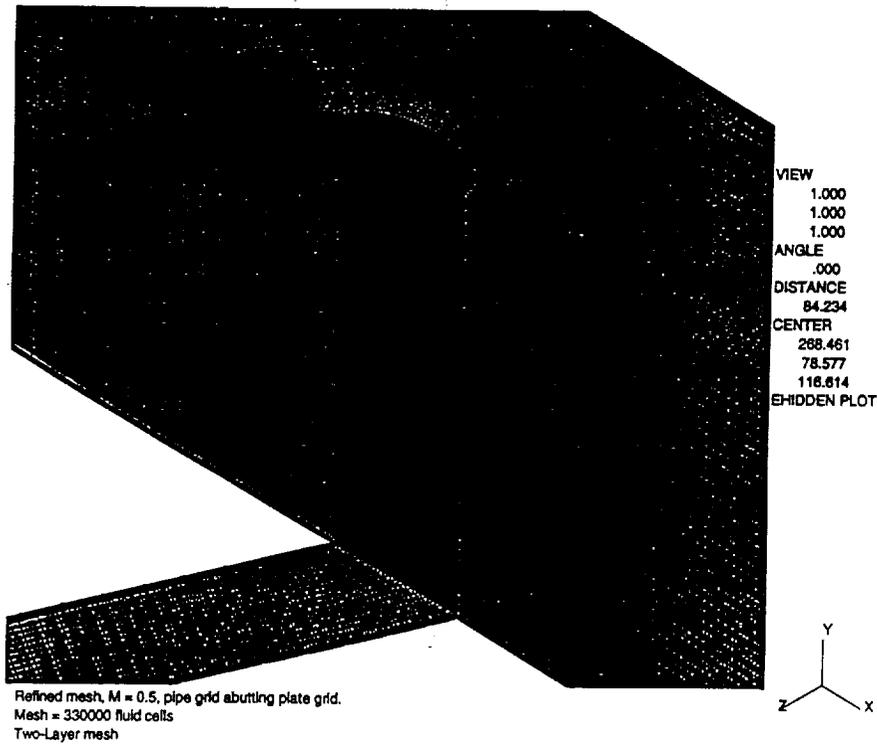
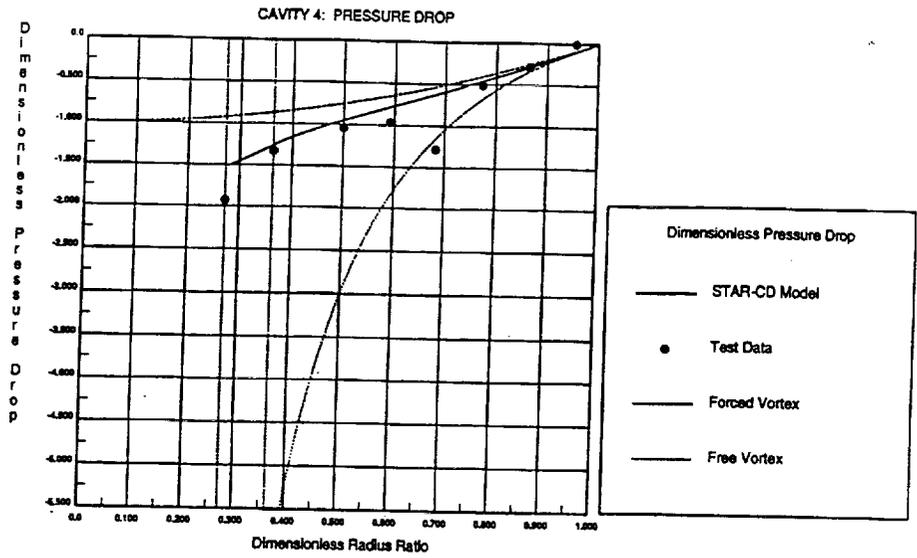
—	36.44
—	33.84
—	31.24
—	28.64
—	26.04
—	23.44
—	20.84
—	18.24
—	15.63
—	13.03
—	10.43
—	7.831
—	5.230
—	2.629
—	0.2792E-01

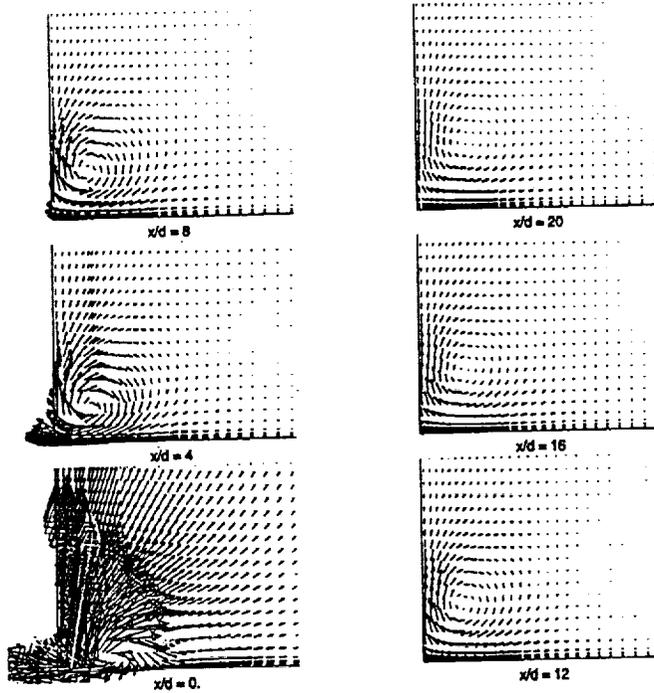
Compressor Drum Test Rig Cold Flow Benchmark Analysis
 Secondary Flow



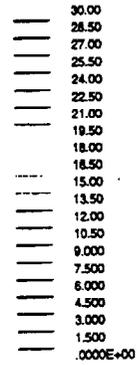
Compressor Drum Test Rig Cold Flow Benchmark Analysis
 Secondary Flow in Cavity 2
 Velocity Vectors at r = 7.40 inches



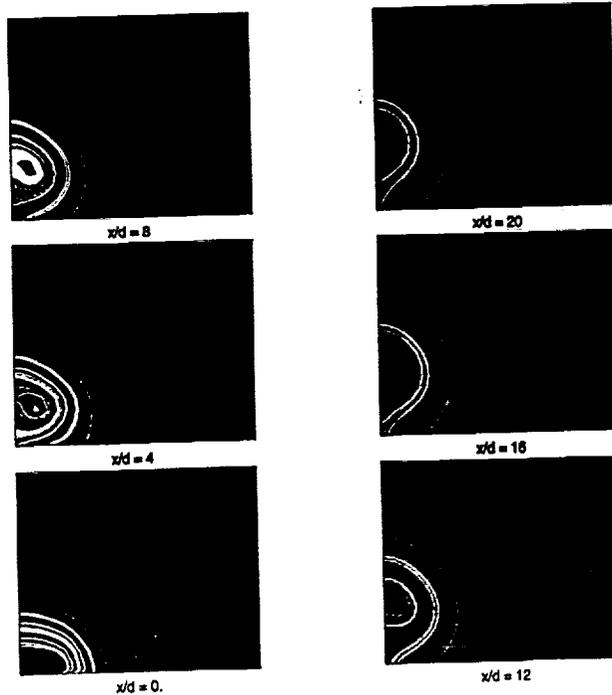




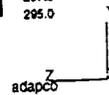
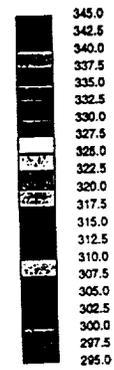
5 Jul 94
 VEL. COMP V W
 M/S
 LOCAL MX= 36.18
 LOCAL MN= .0000E+00



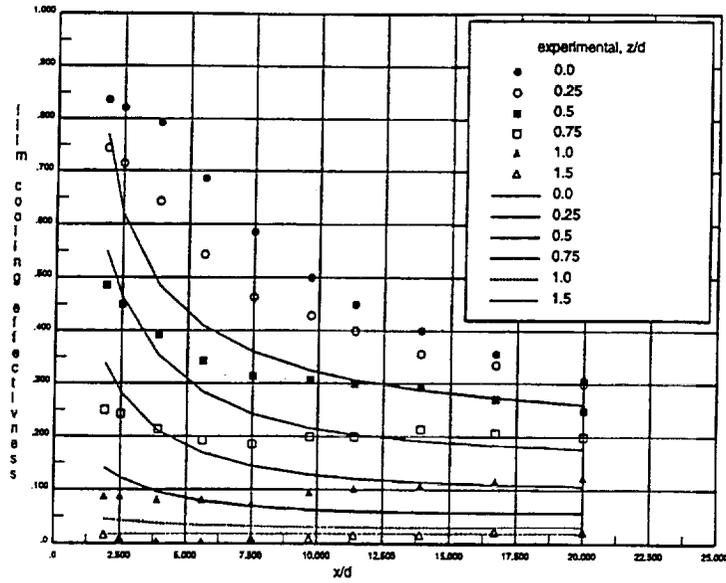
CFD Discrete Hole Film Cooling Verification Study
 Simulation of experiment of Goldstein, et. al. [1968]; Blowing ratio $M=0.5$
 Velocity vectors on spanwise planes; 2-layer model.



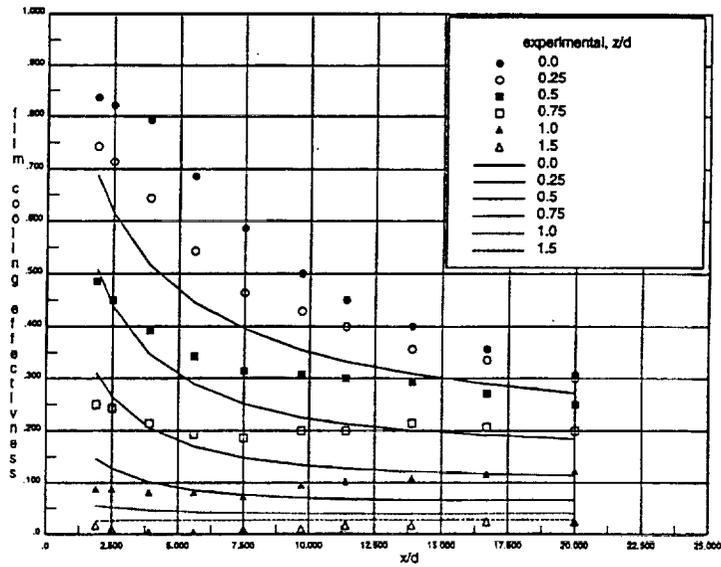
5 Jul 94
 TEMPERATURE
 ABSOLUTE
 KELVIN
 LOCAL MX= 348.9
 LOCAL MN= 292.9



CFD Discrete Hole Film Cooling Verification Study
 Simulation of experiment of Goldstein, et. al. [1968]; Blowing ratio $M=0.5$
 Temperature contours on spanwise planes; 2-layer model.



EXPERIMENTS OF GOLDSTEIN ET AL., 1968
 COMPARISON OF FILM COOLING EFFECTIVENESS
 M = 0.5 : Mesh II.



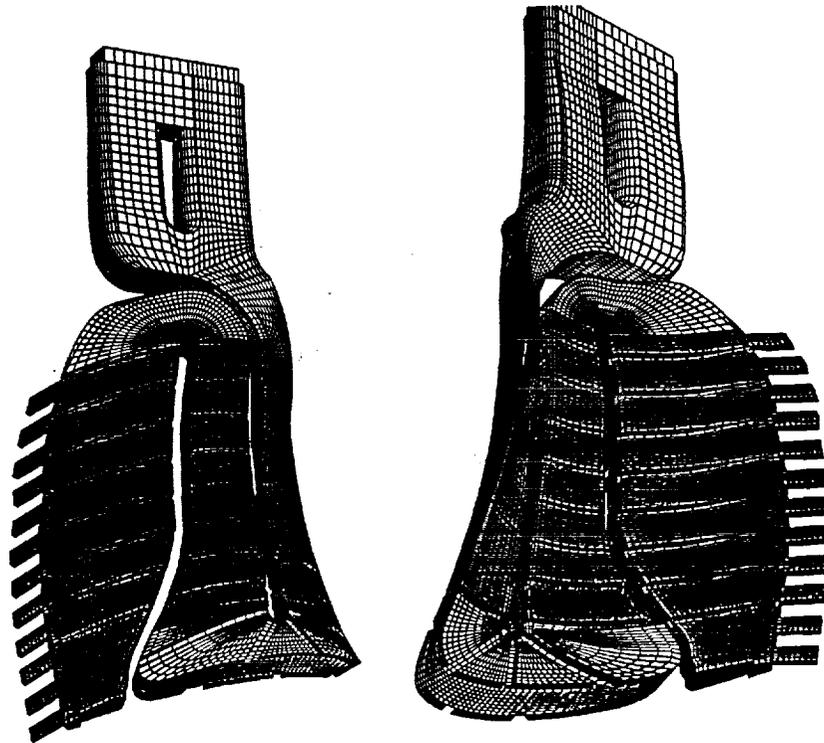
EXPERIMENTS OF GOLDSTEIN ET AL., 1968
 COMPARISON OF FILM COOLING EFFECTIVENESS
 M = 0.5 : 2 Layer mesh.

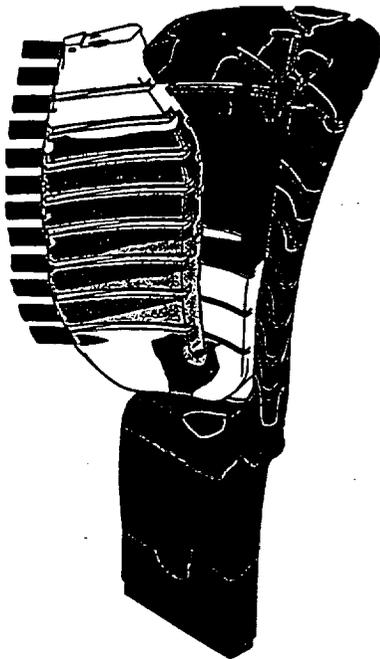
APPLICATIONS & EXPERIENCES (cont'd)

APPLICATION (DATA)	FLOW COMPLEXITY	TURBULENCE MODEL	FINDINGS	T.M. NEEDS
INTERNAL BLADE COOLING ³	<ul style="list-style-type: none"> • FORCE FIELD • B.L. DISRUPTION 	<ul style="list-style-type: none"> • k-ϵ 	<ul style="list-style-type: none"> • DEPENDENCE ON MESH RESOLUTION • GOOD $\Delta P, h$ 	
EXTERNAL CAR AERO-DYNAMICS ⁴	<ul style="list-style-type: none"> • B.L. STRUCTURE INTERACTION • COMPLEX WAKE 	<ul style="list-style-type: none"> • k-ϵ • RNG k-ϵ • 2 LAYER k-l 	<ul style="list-style-type: none"> • DEPENDENCE ON MESH RESOLUTION • GOOD C_D • POOR LIFT 	<ul style="list-style-type: none"> • RSTM • LOW Re RSTM

³GE AIRCRAFT ENGINES [ABUAF & KERCHER (1991)]

⁴10 FORD 1/4 SCALE MODELS IN WIND TUNNEL TEST [WILLIAMS et al (1994)]

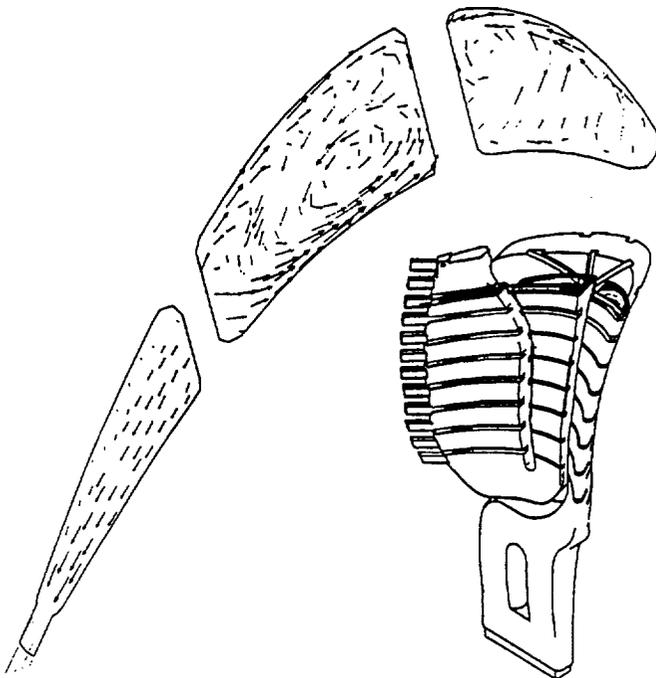
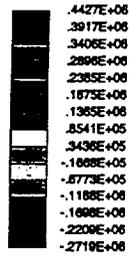




29 Aug 94
PRESSURE

N/M**2

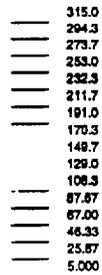
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LOCAL MN= -2719E+06

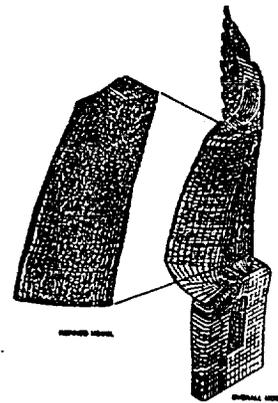
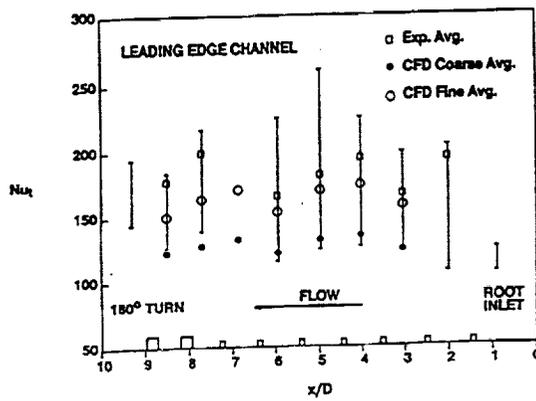
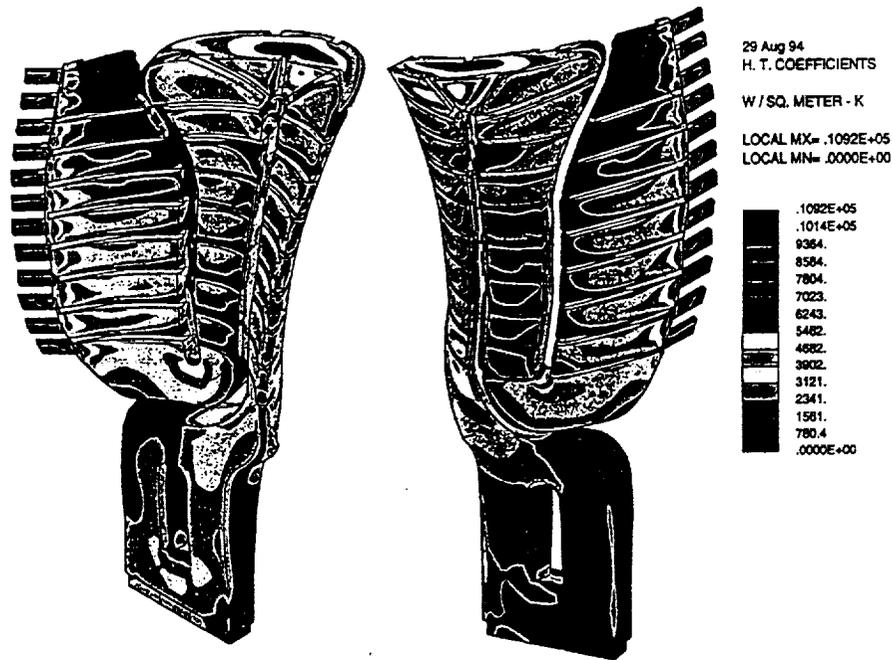


6 Sep 94
MAGNITUDE VELOCITY

M/SEC
PSYS= 2
LOCAL MX= 314.6
LOCAL MN= 4.850

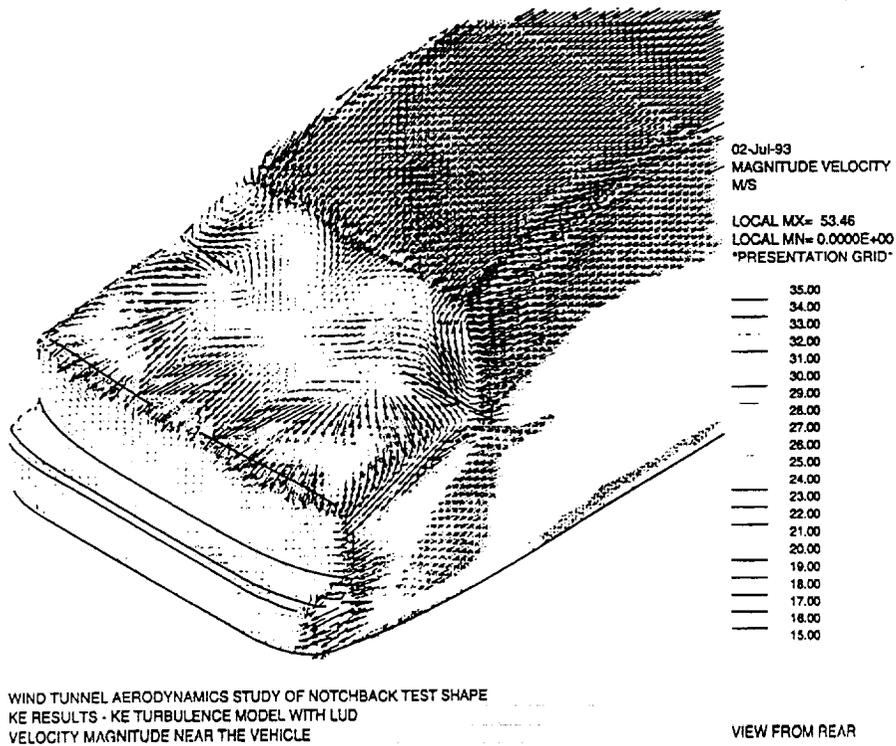
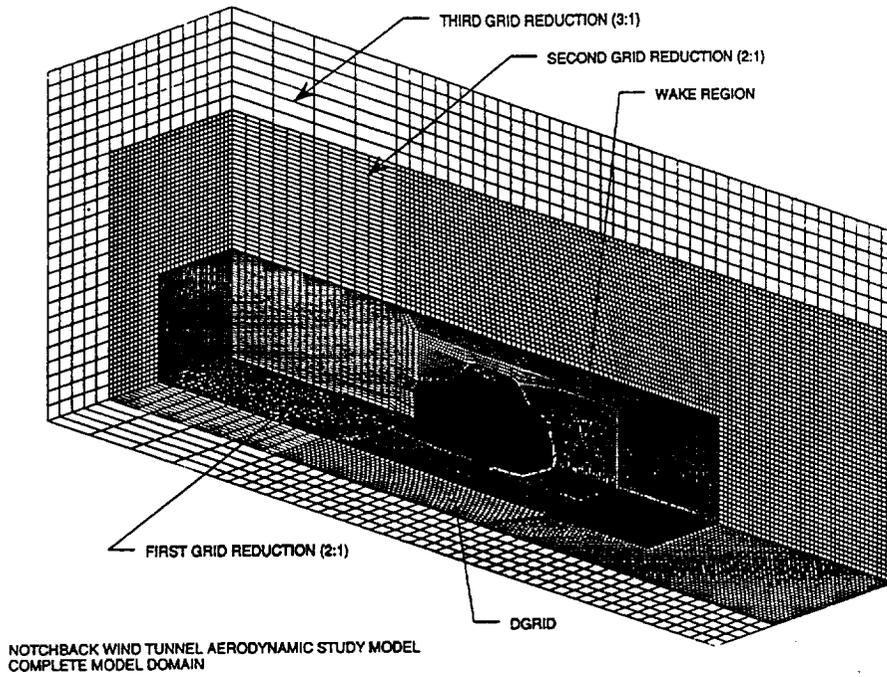
PRESENTATION GRID



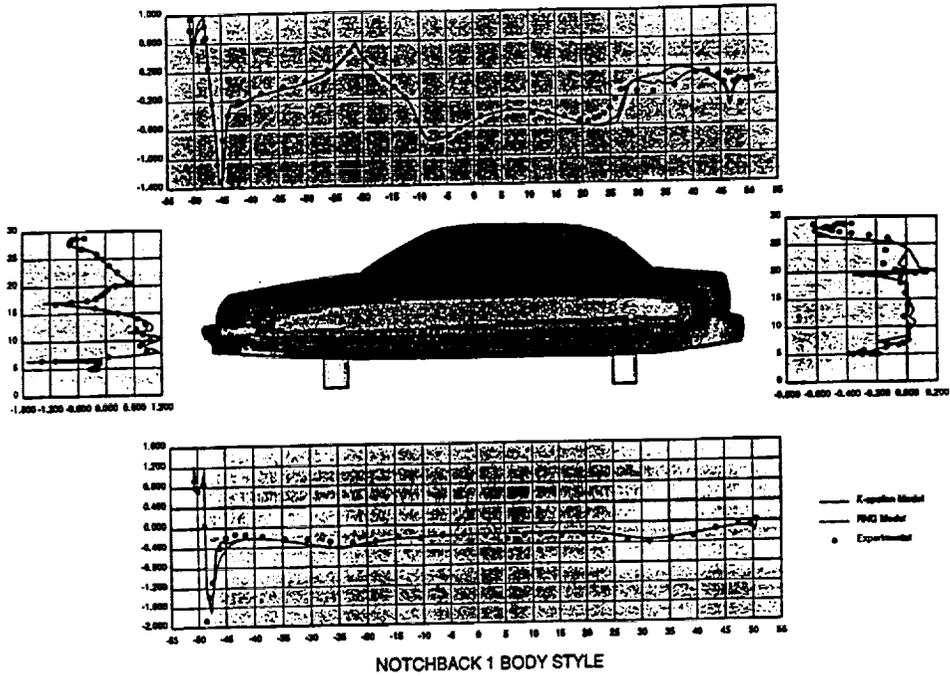


CFD BLADE AND LEADING EDGE MODELS
Marinaccio (1989,1990a,1991)

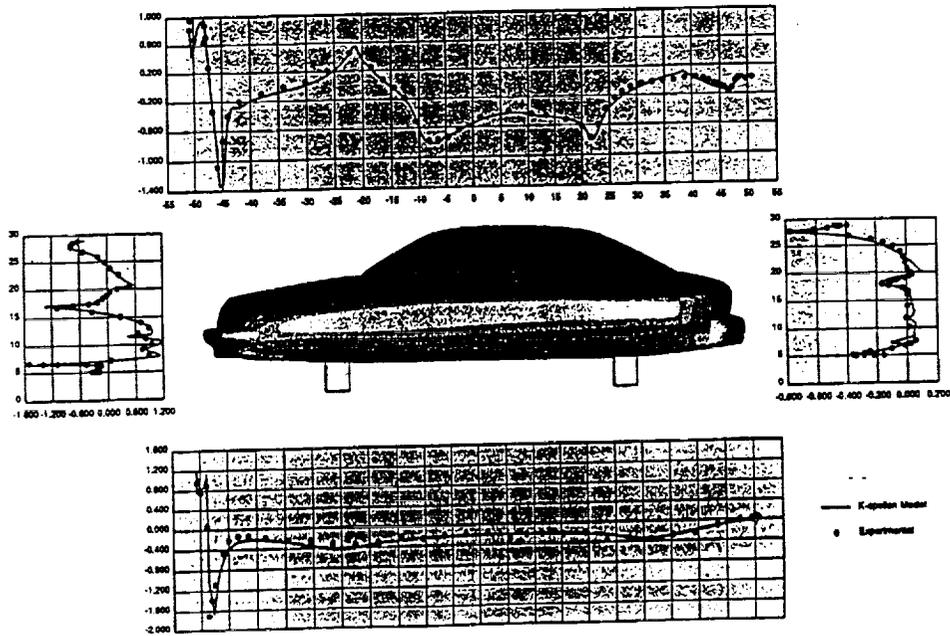
Figure 4 a Leading edge channel heat transfer distribution with distance from the inlet. Comparison of model turbulated convex surface maximum, minimum and average measurements with blade CFD average predictions.

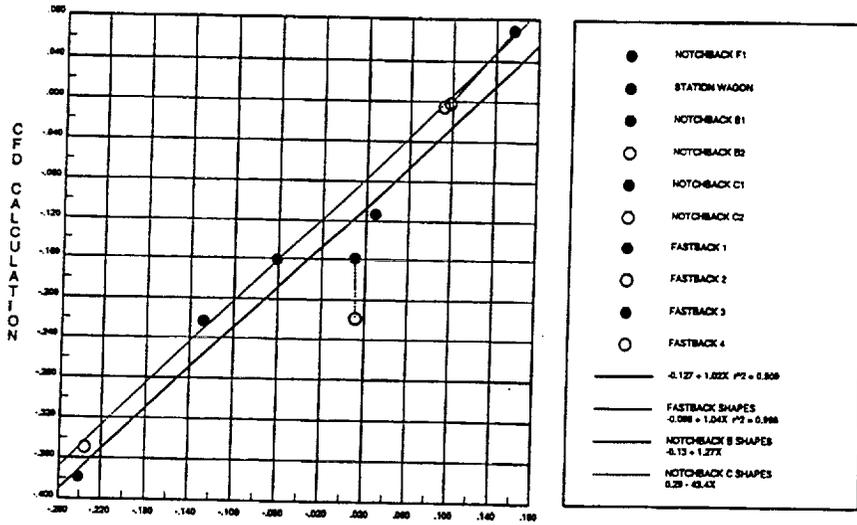


PRESSURE COEFFICIENTS AT THE CENTERLINE OF VEHICLE

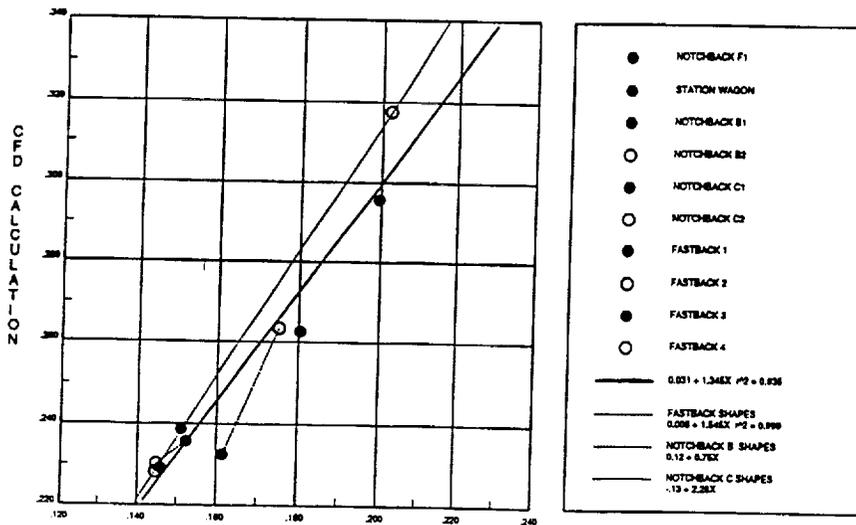


PRESSURE COEFFICIENTS AT THE CENTERLINE OF VEHICLE





EXPERIMENT RESULTS
 COMPARISON OF EXPERIMENTAL AND COMPUTATIONAL LIFT COEFFICIENTS
 K EPSILON TURBULENCE MODEL - *** INITIAL RESULTS ***



EXPERIMENTAL RESULTS
 COMPARISON OF EXPERIMENTAL AND COMPUTATIONAL DRAG COEFFICIENTS
 K EPSILON TURBULENCE MODEL - *** INITIAL RESULTS ***

**CONCLUSIONS: TURBULENCE MODELING
IMMEDIATE NEEDS**

- **NEAR-WALL TURBULENCE**
 - **ECONOMICAL, ROBUST LOW REYNOLDS NUMBER 2 EQ. EVM's AND RSTM**
 - **A GENERAL AND VERSATILE NEAR-WALL TREATMENT FOR RSTM**
- **RSTM MODEL**
 - **ALTERNATIVE CLOSURE OF THE WALL REFLECTION COMPONENT, WITHOUT NEED OF WALL TOPOGRAPHY PARAMETERS**
- **EDDY-VISCOSITY MODELS**
 - **EXTENSION OF THE NON-LINEAR $k-\epsilon$ TO INCORPORATE FORCE-FIELD EFFECTS**
- **BENCHMARKING**
 - **A RELIABLE DATABASE OF BENCHMARK SET OF REPRESENTATIVE COMPLEX FLOWS**
 - **BENCHMARK PERFORMANCE CLASSIFICATION OF VARIOUS EVM's ($k-\epsilon$, $k-\omega$, RNG AND NON-LINEAR $k-\epsilon$, MULTISCALE EVM's) AND RSTM CLOSURE VARIANTS**

**CONCLUSIONS: TURBULENCE MODELING
PROGRAM NEEDS**

- **A LARGER VIEW OF THE RSTM DEVELOPMENT TOWARDS IMPLEMENTATION IN GENERAL COORDINATE, COMPLEX GEOMETRY DOMAIN, UNSTRUCTURED CFD METHOD**
- **A BROADER APPLICATION OF DNS TO COMPLEX FLOWS TO ASSIST TURBULENCE MODEL DEVELOPMENT/OPTIMIZATION**
- **WELL-POSED EXPERIMENTAL DATA, OBTAINED IN THE ORIGINAL OR REDUCED SCALE MODEL OF THE INDUSTRIAL COMPONENT FOR CFD VALIDATION**
- **COLLABORATIVE INDUSTRY-CFD RESEARCH/DEVELOPMENT PROGRAMS FOR EXPERIMENTATION - CFD VALIDATION (CALIBRATION) FOR SPECIFIC INDUSTRIAL APPLICATIONS**

Outline

- Profiles
 - ASC
 - Application
 - Client
- Needs
 - Clients'
 - ASC's
- ASC Directions
 - Research
 - Development
 - Products
- How Can CMOTT Help?

Profile of ASC

- Established in 1985
- Components of business
 - development
 - applications
 - licensing and service
- Geographic markets
 - North America
 - Europe
 - Pacific rim countries

Application Profile

- Rotating machinery components
 - hydraulic turbines
 - pump
 - compressors
 - turbines
 - stators
 - wicket gates
 - scrolls
 - volutes
 - inlets and diffusers
 - seals
 - stage
 - rotor stator

Application Profile cont'd

- Combustion
 - gas turbine combustor
 - coal fired boilers
 - gasification
 - fire suppression
 - emissions reduction
 - safety
- High speed external - ballistics
 - explosively formed projectiles
 - finned projectiles
 - sabot discard
- Heat transfer
 - turbine cooling
 - nuclear reactors
 - heat exchangers
 - electronics system cooling
- Typical uncertainties
 - geometry
 - initial and boundary conditions
 - transient effects
 - transition
 - limitations of physical models
 - numerical error

Client Profile

- Companies or divisions
 - industrial/manufacturing/research
 - 10 - 200 employees
 - limited or no access to high performance computing
- Users
 - design and/or analysis
 - < 3 people
 - network of engineering workstations
 - turnaround time in less than a day for analysis, hours for design

Clients' Needs

Needs are most readily identified through typical questions from clients.

- General
 - I am using $k-\epsilon$ or two-layer or $k-\omega$, or RNG ..., what does it mean to my calculation? Tell me in words what the deficiencies of the model means for my application?
 - What is the relative price/performance of the various turbulence models?
 - Has the model I am using been validated for type of flows I am trying to model? If so, when, where, how ... ?
 - How well does the model handle the interaction between turbulence and rotation, curvature, adverse pressure gradients, separation, swirl, bouyancy, extinction, droplets and particles, anisotropies ...?
 - How can I use Navier-Stokes solvers for design? Can I tune the turbulence model to suit my needs? If so, what are the appropriate settings for my application?

Clients' Needs cont'd

- Grid
 - I don't have access to high performance computing, I don't have any more time, I have a coarse non-orthogonal mesh, is my CFD result useful?
 - I have just made my grid finer, why should I have to worry about whether y^+ is in a given range?
- High speed flows
 - I am solving a flow with many speed regimes including low speed separations and shocks, why do turbulence levels become unphysical as the grid is refined through shocks?
 - How should experimental data be compared to results from time or Favre averaged calculations?

Clients' Needs cont'd

- Combustion
 - Which of the many different combustion models in combination with which turbulence model works best for my application?
 - How appropriate is the single scale implicit in the turbulence model for the combustion model?
 - How can the Bousinesq assumption be valid in the presence of counter-gradient diffusion?
 - How important are turbulent fluctuations to my problem?
 - If I had all the mean flow and fluctuating components of the the turbulent flow, how can the effects of stretch and curvature on the instantaneous flame front be modelled.
 - Can extinction due to vortex stretching be modelled?
 - What is the influence of the flame front on the turbulence?

Clients' Needs cont'd

- Calculated pdf models
 - If I use a more detailed chemistry model - like a pdf transport model - how much improvement can I expect in the results for my application? How can I measure that?
 - Is it the case that the results for my application will not be sensitive to the shape of the pdf? If not, then why should I incur the costs associated with a pdf transport equation.
 - I am solving a pdf transport equation, how much are the results dominated by the limitations of modelling of the diffusion transport term?

Clients' Needs cont'd

- Flamelet models
 - I am using a flamelet model in modelling my gas turbine combustor, but in some regions of the combustor the model is not strictly appropriate - can any of the results be used? If so, how much?
 - In some models like the flamelet model, it is assumed that the turbulent time scale is inversely proportional to the velocity gradient of a "laminar" model flame. What is the validity of this assumption?
 - How sensitive are my results to the assumption of statistical independence of the quantities in a joint pdf?

ASC's Directions

- Develop in-house model expertise
 - two-layer model
 - alternative two-equation models
 - second moment closure models
 - expanded EBU models
 - flamelet model
- Develop in-house expertise applying models
 - turbomachinery
 - combustion
 - heat transfer
- Promote high performance computing
 - parallel computing

How Can CMOTT Help?

- Model improvements to address between turbulence and
 - rotation
 - curvature
 - adverse pressure gradients
 - separation
 - swirl
 - bouyancy
 - droplets and particles
 - anisotropies ...
- as well issues related to
 - extinction
 - trace species
 - vortex stretching
 - flame fronts
 - time and length scales
 - ...
- Great, but is this what users really want?

How Can CMOTT Help? cont'd

- Curator of information on existing models
 - define
 - validate
 - process
 - educate
- as an independent agency

How Can CMOTT Help? cont'd

Define models

- unified conceptual framework
- establish baseline for various models
- set context for model improvements
- for each model
 - > document derivation
 - > identify assumptions
 - > clearly state implications of assumptions
 - > separate physics from numerics

How Can CMOTT Help? cont'd

Validate models

- fundamental flows
 - > validate assumptions
- benchmark problems
 - > select real engineering problems relevant to identified applications (in propulsion)
 - > review selection of benchmark on regular basis
- experimental data
 - > collect and review existing data
 - > define new experiments
 - > review quality of resulting data for validation of models

How Can CMOTT Help? cont'd

Process data

- collect
- distil
- review
- interpret
- describe
- compile

How Can CMOTT Help? cont'd

Educate

- document
- publish
- workshops
- seminars
- short courses
- market

Summary

Provide information so users, for their applications can:

- make an educated choice of model
- understand how to appropriately use existing models
- move forward with existing models and technology
- understand implications of improvements to existing models

SECOND-ORDER CLOSURES FOR COMPRESSIBLE TURBULENCE

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Mechanical and Aerospace Engineering Department
Cornell University
Ithaca, New York

N95- 27898

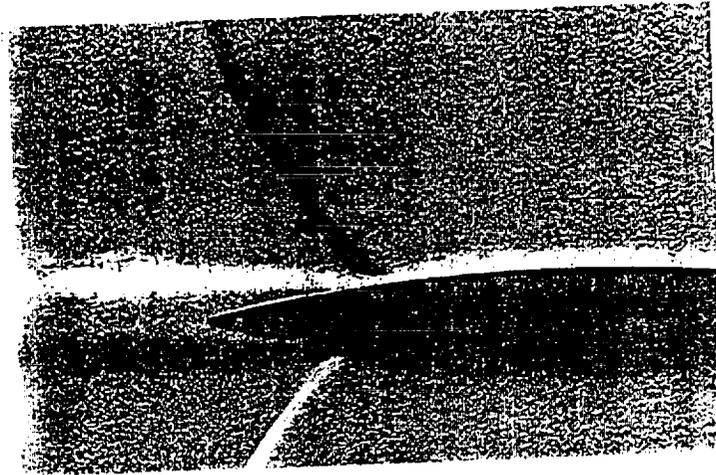
OUTLINE

- I. Project Description
- II. Turbulence Modeling
- III. Computational Engine / Results

FUTURE WORK

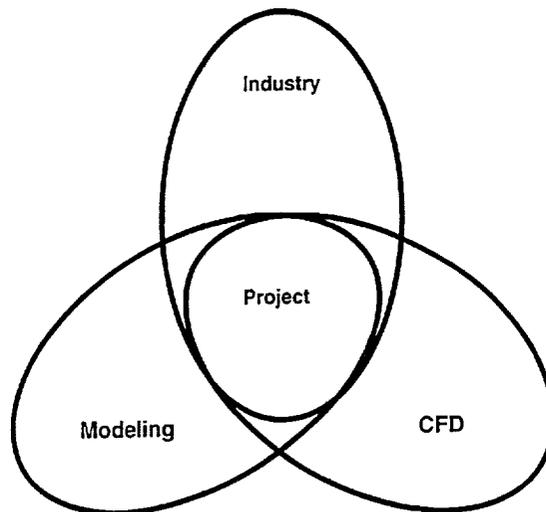
I. PROJECT DESCRIPTION

1. Flows of Interest
2. Motivation
3. Method



Schlieren photograph of a shock-wave turbulent boundary-layer interaction
 $M=0.90$ $Re=1,750,000$ [Liepmann]

1.2.MOTIVATION



- Physics
 - Boundary Layer Separation & Wall Heat Transfer
 - Spreading rate

- Modeling
 - Account for Compressibility Effects on Turbulence

- Numerics
 - Compare 1-point Closures on Identical Solver

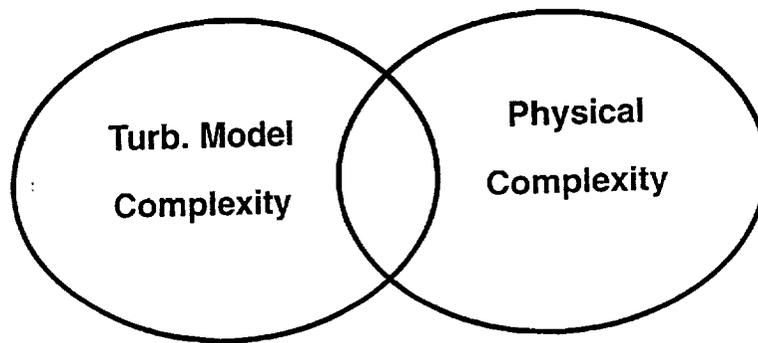
I.3. METHOD

- 1-Point Closures: from EVM to Second-Order Closures

- Dynamical Compressibility Effects

- 3D / Finite Volume Approach

II. TURBULENCE MODELING



1. Closure Levels
2. Compressibility Effects
3. Shock Wave Interactions

II.1. Closure Levels

1. EVM Mixing-Length
(Baldwin-Lomax)
2. EVM Multi-Equation
(k - ϵ - S)
3. Second-Order Closure
(Shih and Lumley)

II.2. Compressibility Effects

1. New Physics & Averaging
2. Models

II.2.1. New Physics (Turbulent Kinetic Energy Sink)

$$- \langle \tau_{ij} u_{i,j} \rangle = \Pi_d - \epsilon_d - \epsilon_s$$

- $\epsilon_d = (\mu_B + \frac{4}{3}\mu) \langle d^2 \rangle$
- $\Pi_d = \langle pd \rangle$

II.2.3. Turbulence Modeling (Zeman, Sarkar et al., Yoshizawa)

- dilatation dissipation:

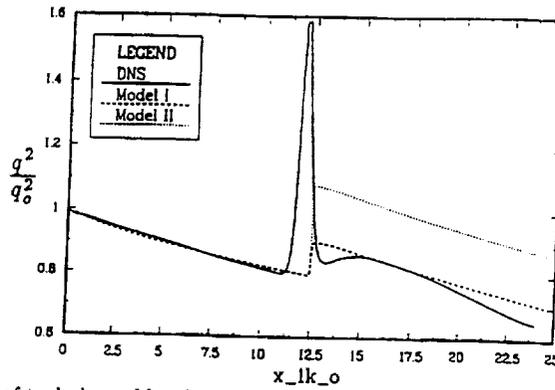
$$\epsilon_d = (\mu_B + \frac{4}{3}\mu) \langle d^2 \rangle$$

- Sarkar et al. (asymptotic analysis)
- Zeman
(Shocklet model)

- pressure-dilatation correlation:

$$\Pi_d = \langle pd \rangle$$

- Zeman (acoustic model):
- Sarkar et al.
(DNS & asymptotic analysis)



Response of turbulence kinetic energy to the passage through shock

II.3. Shock Wave Interactions

1. Experimental Observations
2. Physics
3. Modeling

II.3.1. Experimental Results

- Oscillation increases with Shock Strength (Dolling)
- Oscillation increases with Separation Region
- Normal Stresses Preferentially Amplified (Délery et al.)

II.3.2. Physics

Oscillation Caused by (?):

- "Breathing" of Separation Region
- Vortex Bursting
in Incoming Boundary Layer
(Dolling)

II.3.3. Shock Oscillation Modeling

- Parametrized Source Terms
in Normal RS Evolution Equation
(gradient activated)
- Separation region Extend

III. COMPUTATIONAL ENGINE

1. Numerical Method
2. Turbulence Models
3. Validation Procedure / Results

III.1. Numerical Method

Initial Code: flo103 (A. Jameson L. Martinelli, Princeton)	Current Code: cyste (D. Caughey)	Future
1. Geometry C-mesh 2D	1. Geometry O- R-meshes (EAGLEView MSU)	1. Geometry 3D
2. PDE Solver spatial discretization: FV time integration: RK	2. PDE Solver variable number of PDE's consistent gradient comp.	2. Turbulence Models SOC
3. Convergence Acceleration: variable time step residual smoothing artificial dissipation multigrid preconditioning	3. Convergence Acceleration Enhanced multigrid sequencing	
4. I/O PLOT3D format	4. I/O Restart option Post-processing (DX, Tecplot,...) convergence histories	
5. Turbulence Models Baldwin-Lomax	5. Turbulence Models k-epsilon (-S)	
	6. Software Engineering Dynamical mem. allocation (C) Vectorized data structure Unix Integration	

III.2. Turbulence Models:

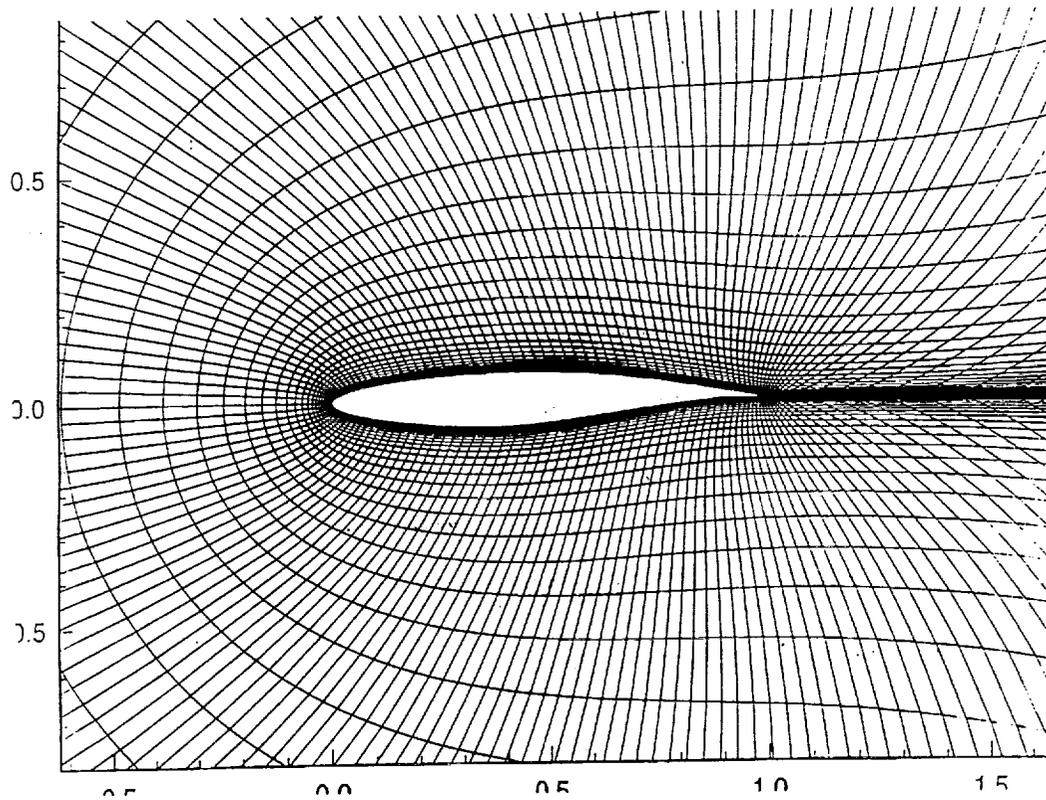
Incompressible / Compressible: an additive approach

- Baldwin-Lomax
- k-Epsilon / k-Epsilon-S: B.C's
- Second-Order Closures

Boundary Conditions: Wall-Functions

III.3. Validation Procedure / Results

- Calibration against simple well-documented flows (flat plate, jet)
- Results and Comparison of models



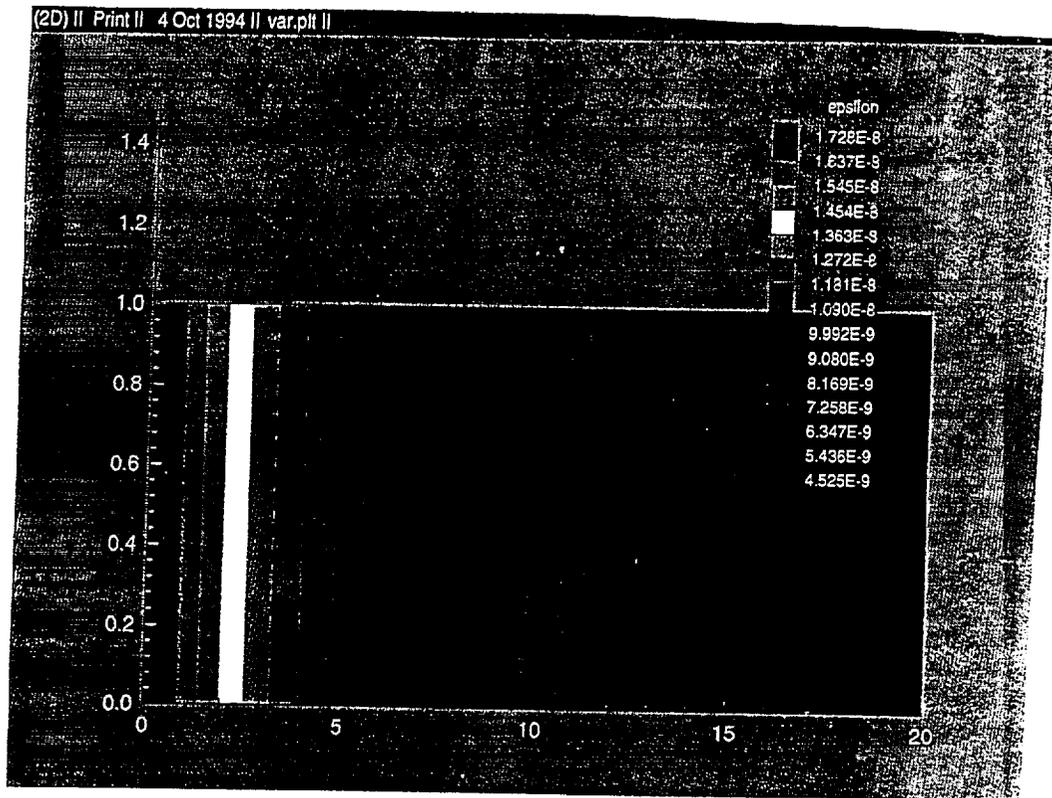
FUTURE WORK

- Numerics

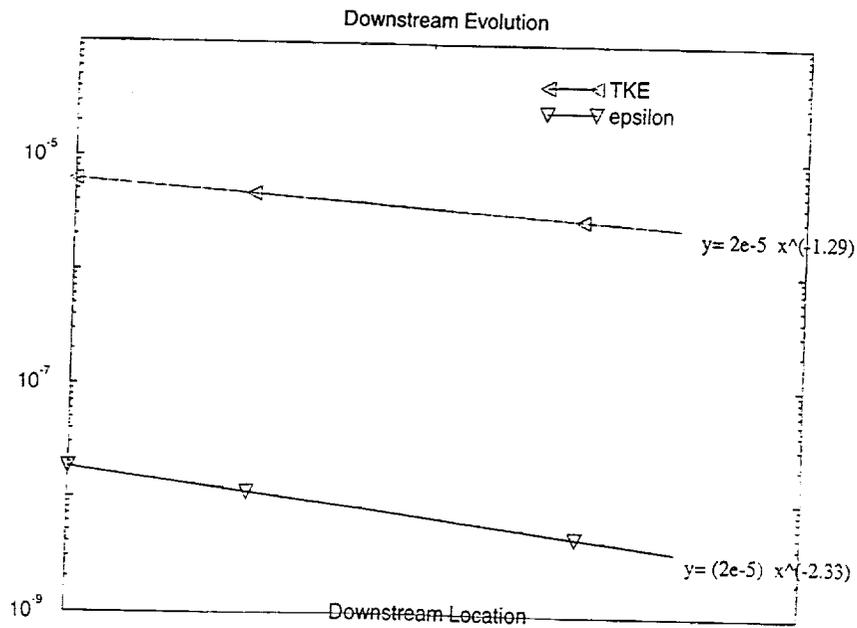
- 2D \Rightarrow 3D
- More Complex Wall Functions
- Realizability Conditions (SOC)

- Modeling

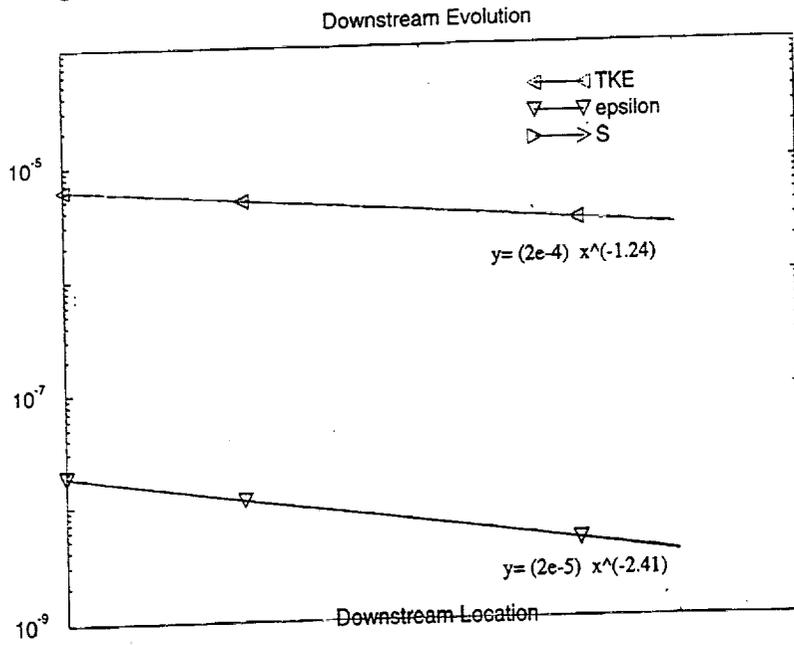
- Refinement of Existing Models (ϵ_d , $\langle pd \rangle$)
- Shock Oscillation Model



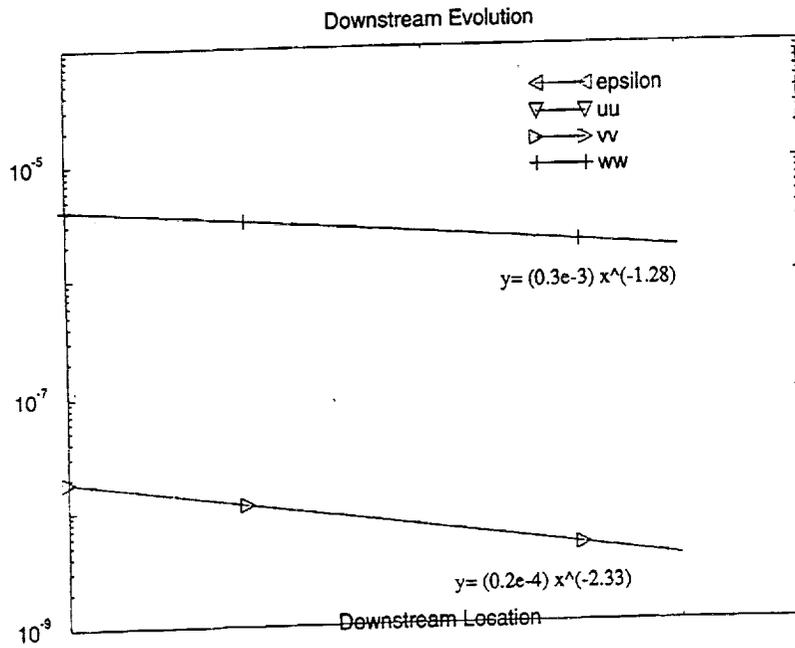
Homogeneous Turbulence (R) / k-eps / Mach=0.045 Re=24357



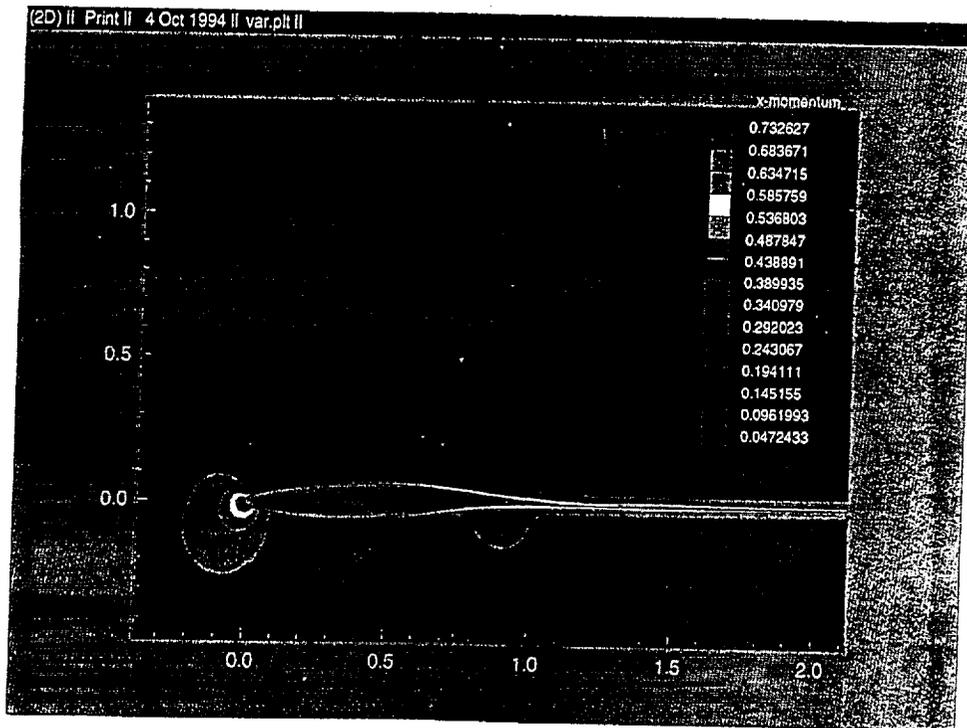
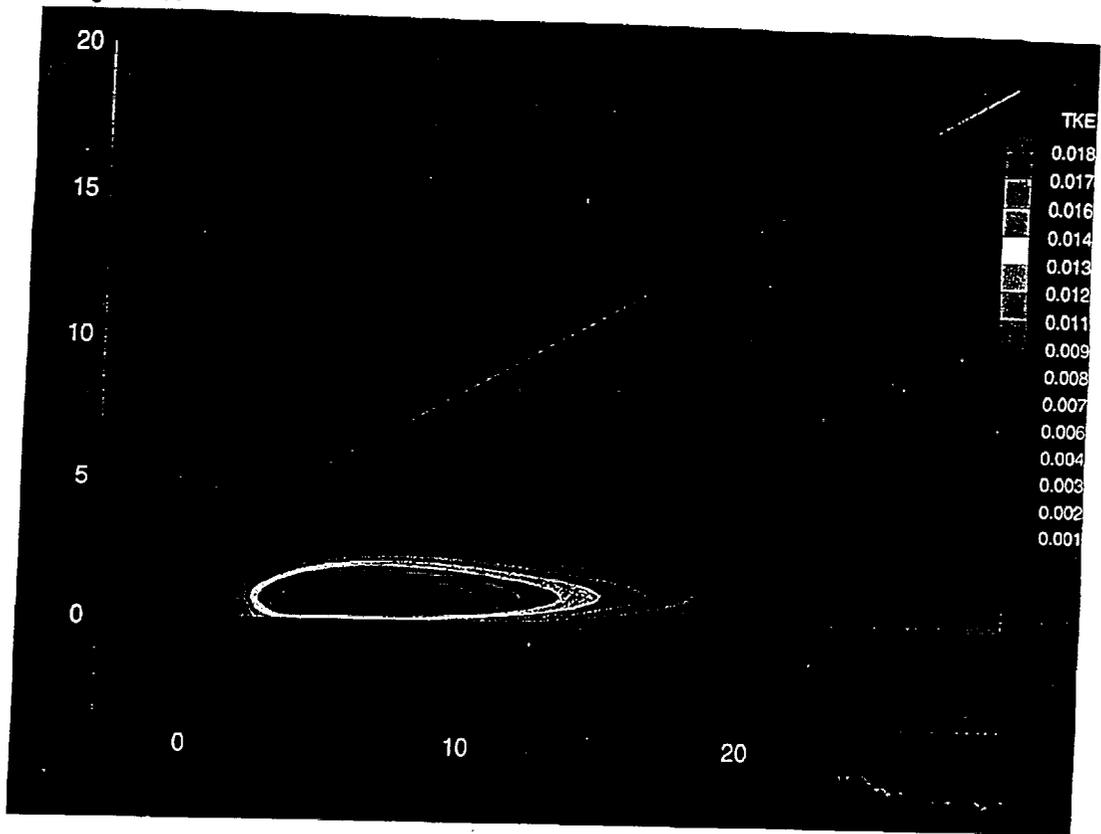
Homogeneous Turbulence (R) / k-eps-S / Mach=0.045 Re=24357



Homogeneous Turbulence (R) / RSC / Mach=0.5

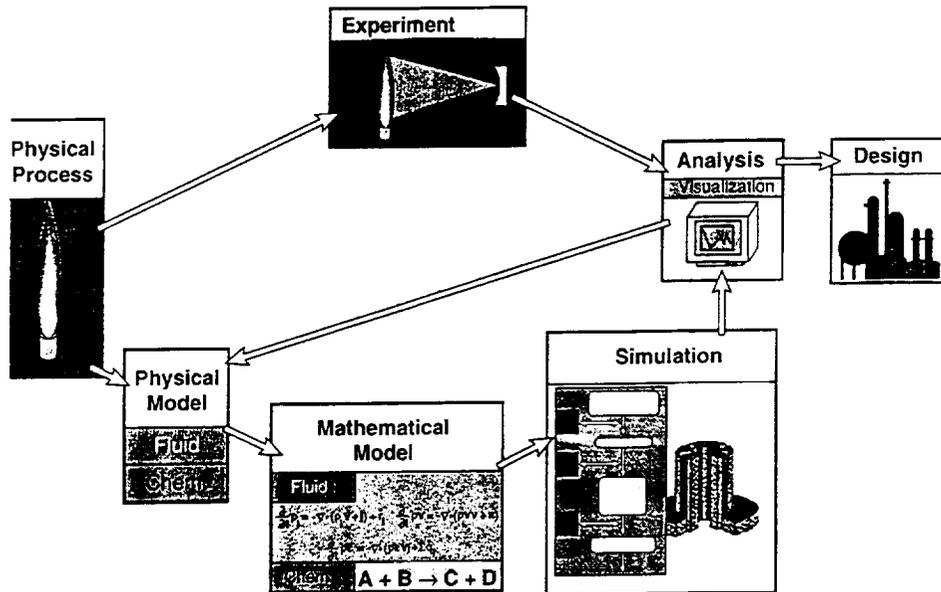


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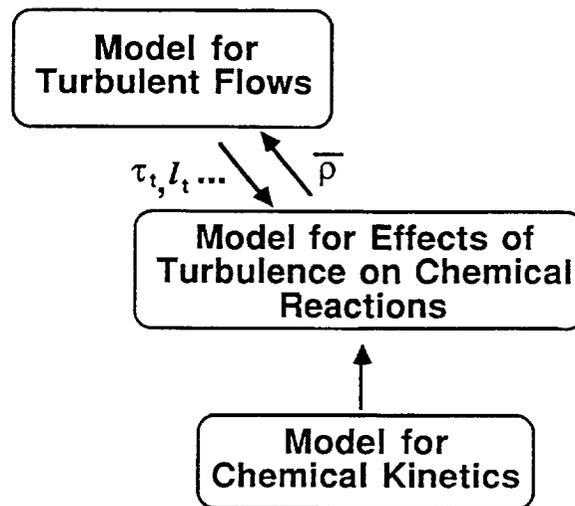




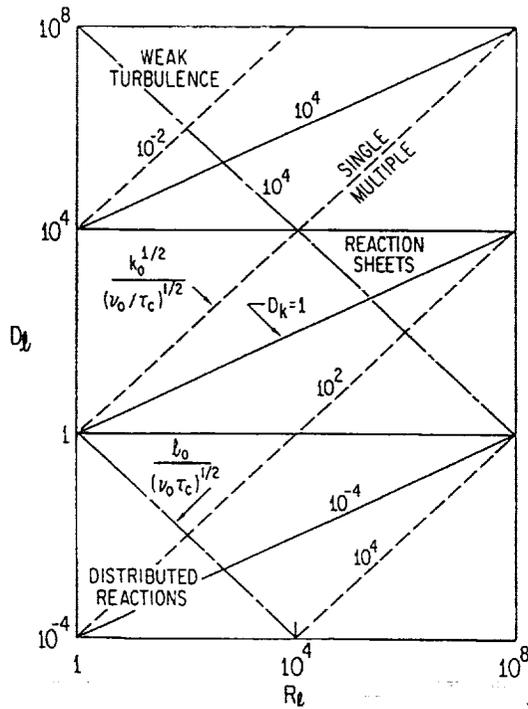
J.-Y. Chen
 Department of Mechanical Engineering
 University of California, Berkeley
 Berkeley, California



Modeling Turbulent Reacting Flows

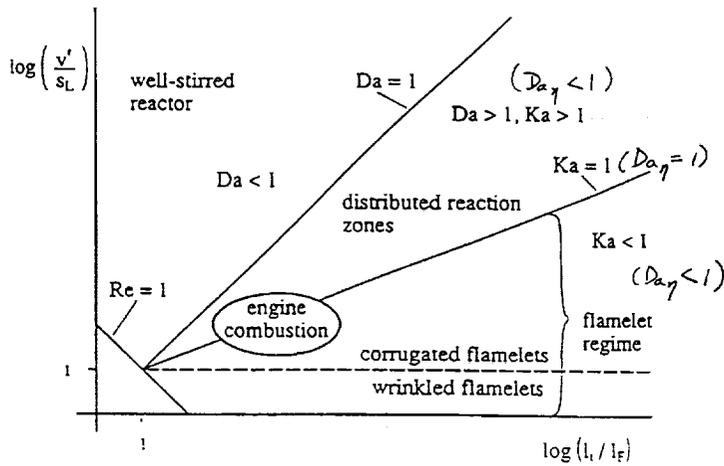


Regimes of Turbulent Combustion



Turbulent Reactive Flows edited by P.A. Libby and F.A. Williams (1994)

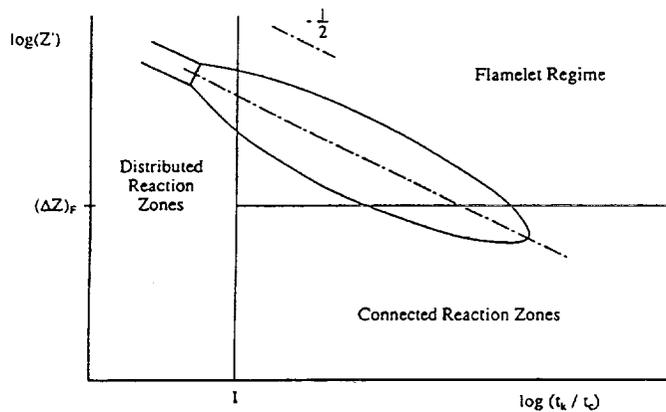
Regimes of Premixed Turbulent Combustion



$$Ka = 1 / Da_\eta$$

Turbulent Reactive Flows edited by P.A. Libby and F.A. Williams (1994)

Regimes of Non-Premixed Turbulent Combustion



Turbulent Reactive Flows edited by P. A. Libby and F. A. Williams (1994)

Chemical Closure Models

(1) Laminar Chemistry

$$\langle \rho w_i \rangle = \rho w_i(\bar{Y}_i, \bar{T})$$

(2) Fast Chemistry

$$\langle \rho w_i \rangle \approx -\frac{1}{2} \bar{\rho} \tilde{\chi}_f \frac{\partial^2 Y^e(f)}{\partial^2 f}$$

(3) Flamelet model

$$\langle \rho w_i \rangle = \iint \rho w_i(\eta, \chi_f) P_{f, \chi_f}(\eta, \epsilon_f) d\eta d\epsilon_f$$

(4) Assumed PDF:

$$\langle \rho w_i \rangle = \int \dots \int \rho w_i(\phi_i) \cdot P_\phi d\phi_1 d\phi_2 \dots d\phi_n$$

Assumed the shape of P_ϕ .

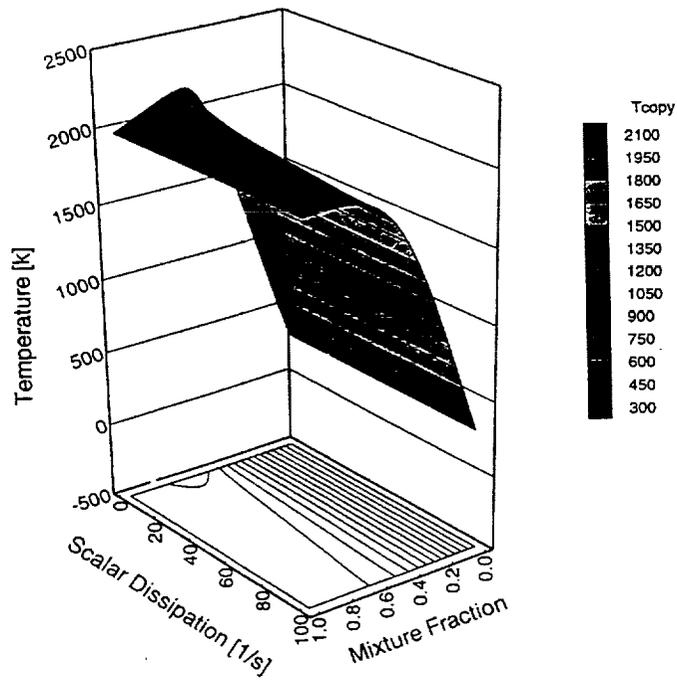
(5) Scalar PDF method:

Solve for P_ϕ directly.

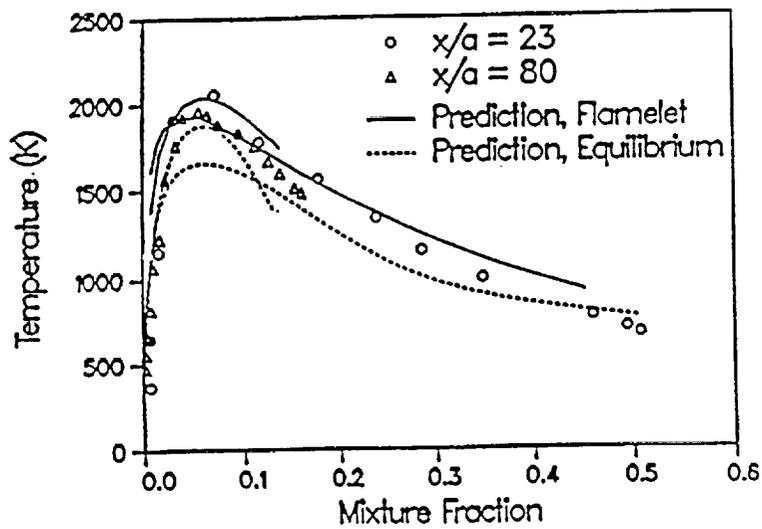
(6) Conditional Moment Closure (CMC)

$$\langle \rho w_i \rangle = \int \langle \rho w_i | \eta \rangle \cdot P_f(\eta) d\eta$$

Flamelet library with one side being burned premixed flame $\phi=1.4$

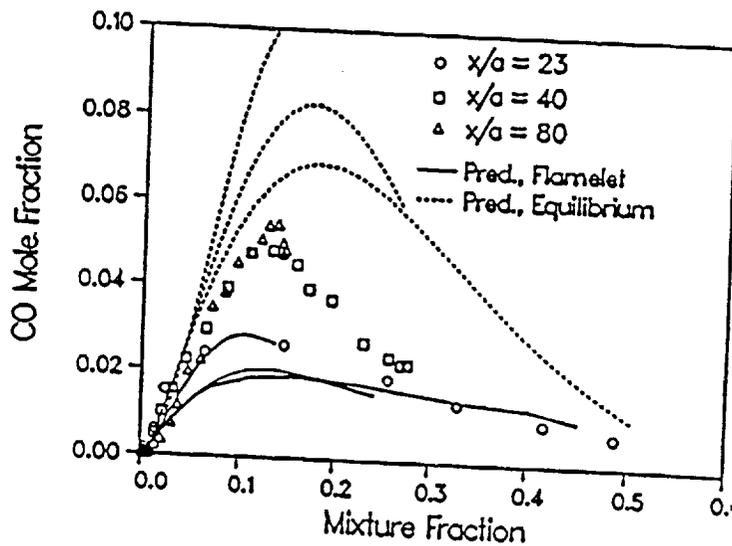


Flamelet Model: 69% H_2 +31% CH_4
Turbulent Jet Flame, $Re_\tau=10,000$



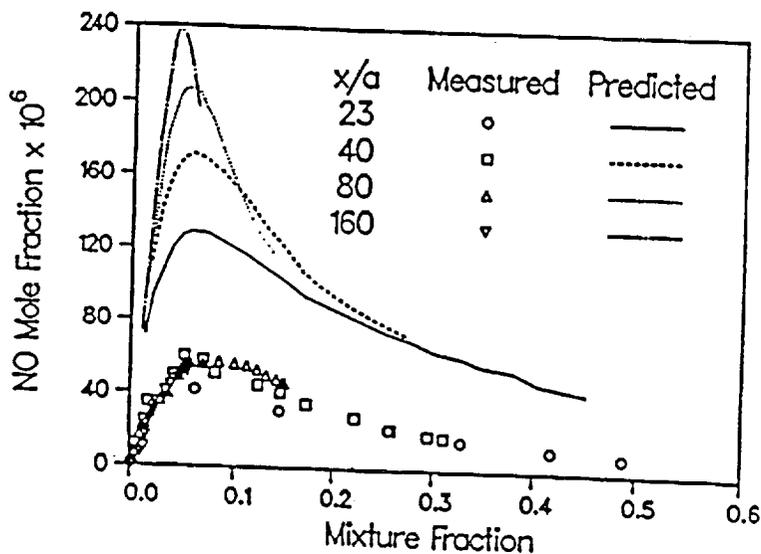
Vranos, et al. "Nitric Oxide Formation and Differential Diffusion in a Turbulent Methane-Hydrogen Diffusion Flame," 24th Symposium (International) on Combustion/The Combustion Institute, 1992/pp. 377-384

Flamelet Model: 69%H₂+31%CH₄
Turbulent Jet Flame, Rey.=10,000



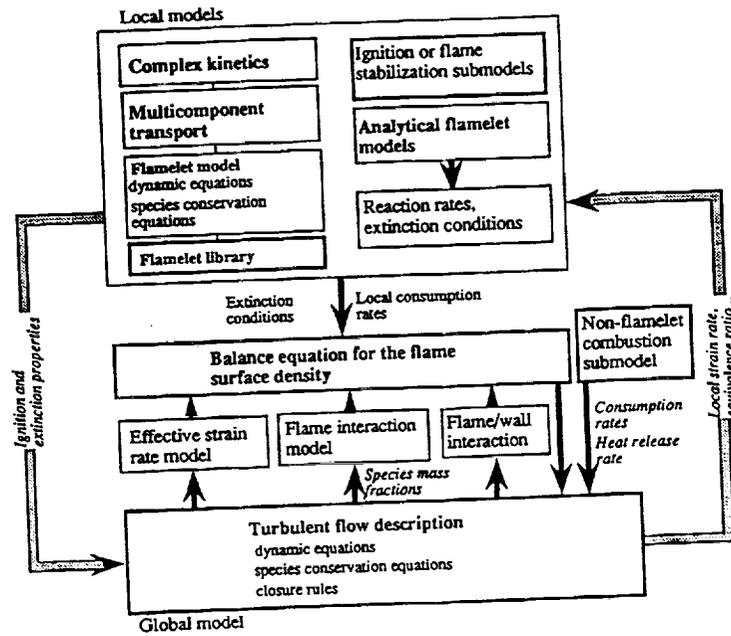
Vranos, et al. "Nitric Oxide Formation and Differential Diffusion in a Turbulent Methane-Hydrogen Diffusion Flame," 24th Symposium(International) on Combustion/The Combustion Institute, 1992/pp. 377-384

Flamelet Model: 69%H₂+31%CH₄
Turbulent Jet Flame, Rey.=10,000



Vranos, et al. "Nitric Oxide Formation and Differential Diffusion in a Turbulent Methane-Hydrogen Diffusion Flame," 24th Symposium(International) on Combustion/The Combustion Institute, 1992/pp. 377-384

Advanced Flamelet Approach



Conditional Moment Closure (CMC)

Definition:

$$\langle Y_i | \eta \rangle \equiv \langle Y(\bar{x}, t) | f(\bar{x}, t) = \eta \rangle$$

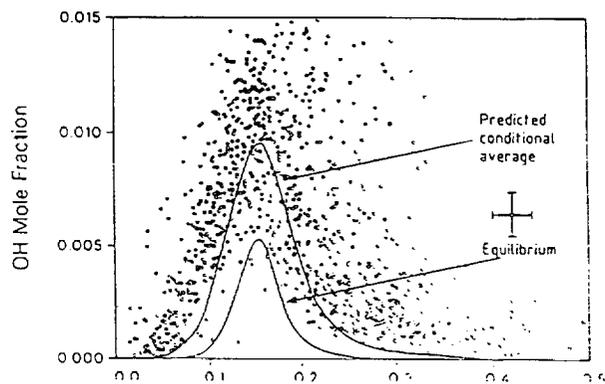
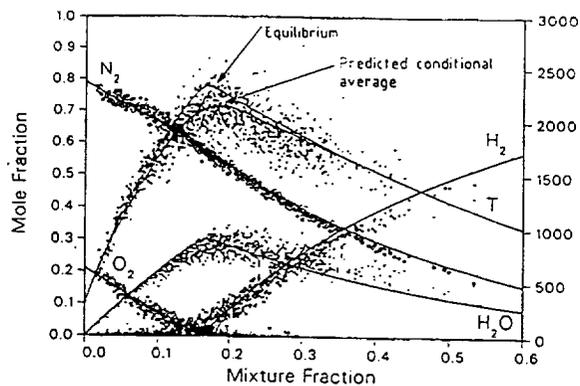
Equation:

$$\begin{aligned} \langle \rho | \eta \rangle \frac{\partial \langle Y_i | \eta \rangle}{\partial t} + \langle \rho \bar{u} | \eta \rangle \cdot \nabla \langle Y_i | \eta \rangle + \frac{\nabla \cdot \{ \langle \rho u' y' | \eta \rangle P_i(\eta) \}}{P_i(\eta)} \\ = \langle \rho w_i | \eta \rangle + \langle \rho D_i \nabla f \cdot \nabla f | \eta \rangle \frac{\partial^2 \langle Y_i | \eta \rangle}{\partial \eta^2} \end{aligned}$$

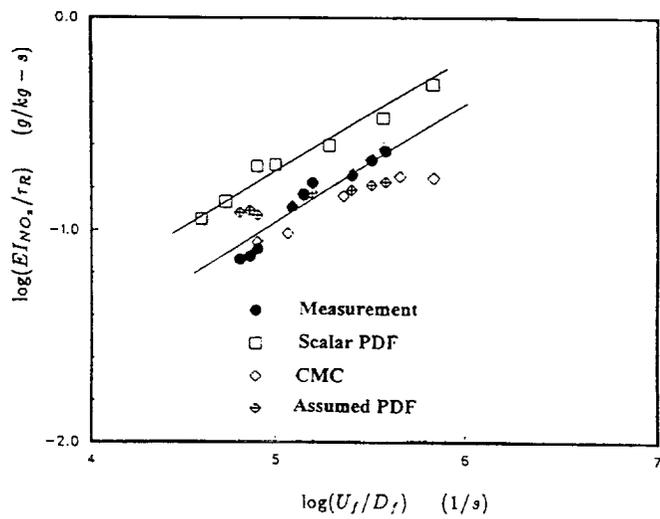
Modeling:

$$\begin{aligned} \langle w_i | \eta \rangle &\approx w_i(\langle T | \eta \rangle, \langle Y_i | \eta \rangle, \dots) \\ \langle \rho D_i \nabla f \cdot \nabla f | \eta \rangle &\approx \langle \rho D_i \nabla f \cdot \nabla f \rangle \approx \frac{1}{2} \bar{\rho} \chi_i \\ \langle \rho \bar{u} | \eta \rangle &\approx \bar{\rho} \bar{u} \\ \langle \rho u' y' | \eta \rangle &\approx 0 \\ \langle \rho | \eta \rangle &\approx \rho(\langle Y_i | \eta \rangle, \langle T | \eta \rangle) \end{aligned}$$

Conditional Moment Closure (CMC)



NOx Emissions from Turbulent H2 Jet Flames



Conditional Moment Closure (CMC)

Applications:

- **Incorporated into existing moment closure CFD codes for complex geometry flows**
- **Realistic Chemistry - Detailed or reduced**

Research issues:

- **Modeling of conditional statistics**
- **Preferential diffusion**
- **Parallel computing algorithms**

Probability Density Function (PDF)

Applications:

- **NO_x from methane jet flames with reduced chemistry**
- **Sooting flames**
- **2-D flows**

Research Topics:

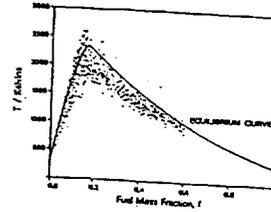
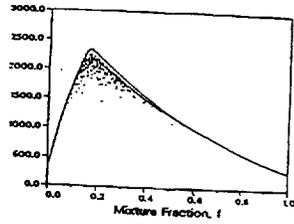
- **Mixing model**
- **Extension to droplet spray & particle laden flows**
- **Preferential diffusion**
- **Efficient stochastic algorithm**
- **Construction of chemical tables**
- **Parallel computing - 3D Flows or 2D flows with complex chemistry**

Departures From Chemical Equilibrium

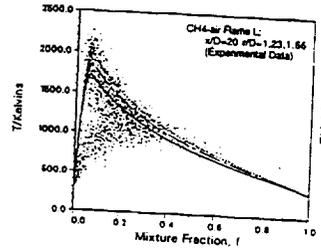
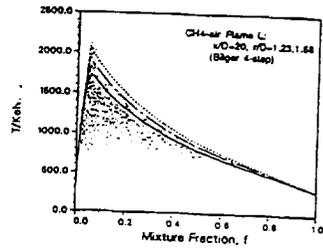
(PDF)

Hydrogen

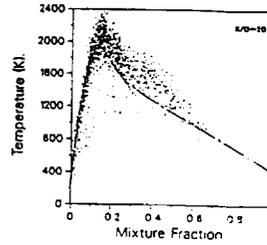
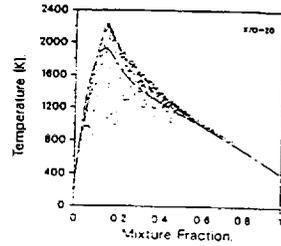
(EXP)



Methane



Methanol



Mixing Models for PDF Methods

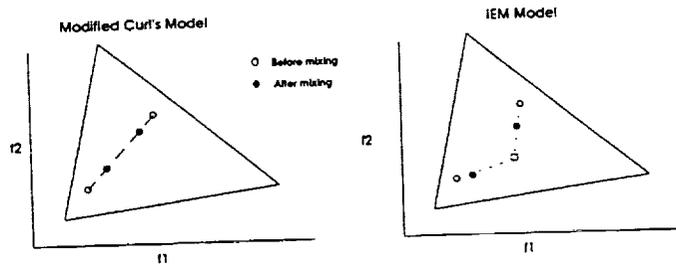
- Modified Curl's Model (stochastic)

$$-\sum_{\alpha=1, \beta=1}^k \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left\{ \left\langle \varepsilon_{\alpha\beta} \middle| \bar{\phi} = \bar{\psi} \right\rangle \bar{P}_\phi(\bar{\psi}, t) \right\} = \frac{1}{\tau_{mix}} \left\{ \iint_{\psi' \psi''} \left[\bar{P}_\phi(\psi', t) \bar{P}_\phi(\psi'', t) H(\psi', \psi'' | \bar{\psi}) - \bar{P}_\phi(\bar{\psi}, t) \right] d\psi' d\psi'' \right\}$$

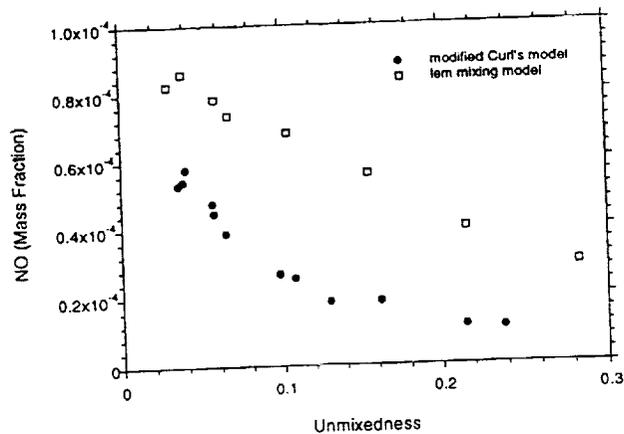
- IEM (Interaction-by-Exchange-with-the-Mean) Model (deterministic)

$$-\sum_{\alpha=1, \beta=1}^k \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left\{ \left\langle \varepsilon_{\alpha\beta} \middle| \bar{\phi} = \bar{\psi} \right\rangle \bar{P}_\phi(\bar{\psi}, t) \right\} = \frac{C_\phi}{2\tau_{mix}} \frac{\partial}{\partial \psi_\alpha} \left[(\bar{\psi} - \bar{\phi}) \bar{P}_\phi(\bar{\psi}, t) \right]$$

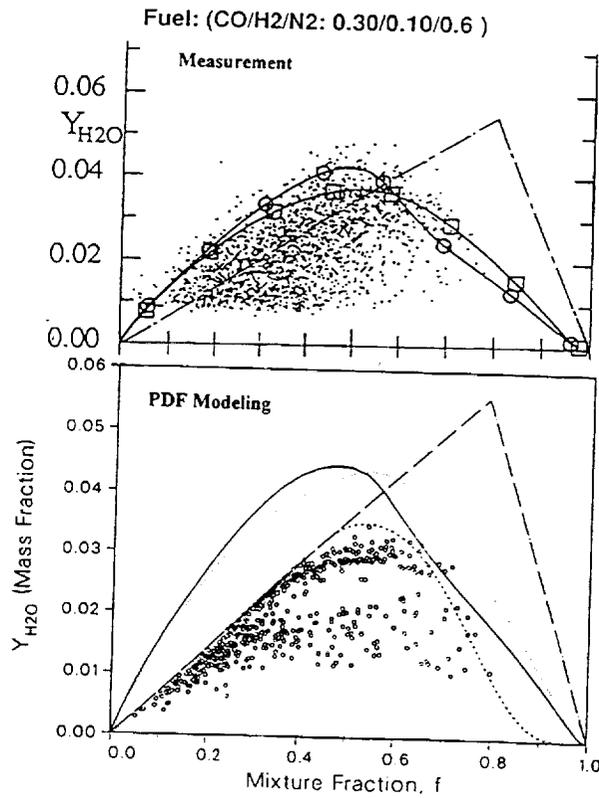
Mixing Frequency: $\omega_{mix} = 1/\tau_{mix}$



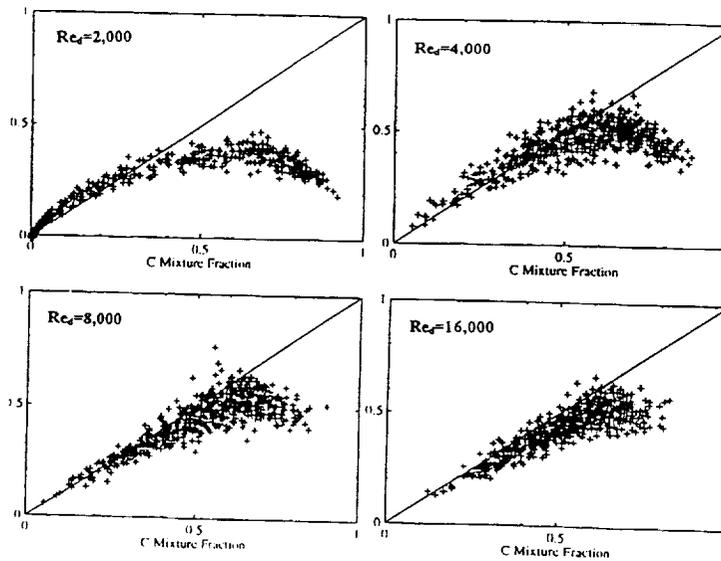
PaSR: H₂/NO_x Detailed Chemistry $\phi=1$ $\tau=1$ ms



Comparison of Predicted and Measured H₂O Mass Fractions Turbulent Nonpremixed Jet Flames

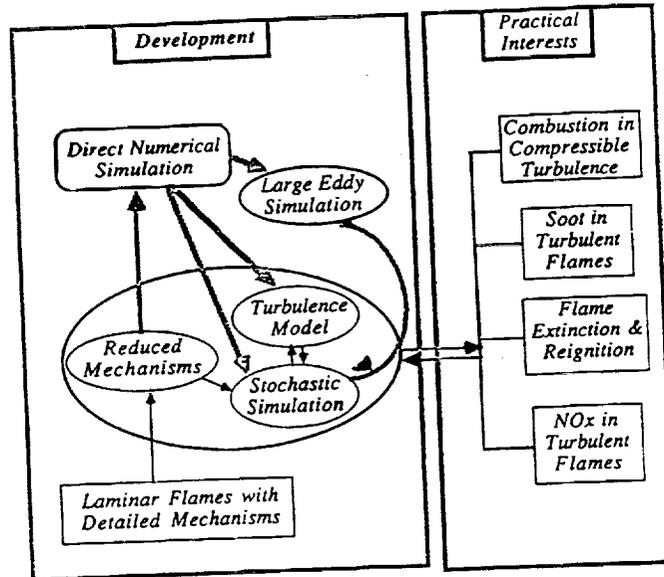


Experimental Evidence of Preferential Diffusion in Turbulent Jet Flames (Fuel: 36% H₂ + 64% CO₂)



"Differential Molecular Diffusion in Reacting and Nonreacting Turbulent Jets of H₂/CO₂ mixing with Air." L.L. Smith Ph.D. Thesis, University of California at Berkeley (1994)

Computation of Turbulent Reacting Flows



INTRODUCTION TO TURBULENCE SUBPROGRAM

T.-H. Shih and J. Zhu
Institute for Computational Mechanics in Propulsion
and Center for Modeling of Turbulence and Transition
NASA Lewis Research Center
Cleveland, Ohio

OBJECTIVES

- A means for CMOTT to interact with industry
- A vehicle for technology transfer to industry

CONCEPT OF TURBULENCE MODULE

- Exact CFD equations:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) - \rho \overline{u_i u_j} \right] - \frac{\partial P}{\partial x_i}$$

- Reynolds stresses will be recasted as:

$$-\rho \overline{u_i u_j} \equiv \underbrace{\mu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right)}_{T_{ij}} + \underbrace{[-\rho \overline{u_i u_j} - \mu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right)]}_{T_{ij}}$$
$$\mu_T \equiv C_\mu \frac{k^2}{\varepsilon}$$

- CFD equations become:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} \left[(\mu + \mu_T) \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) \right] + \frac{\partial T_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i}$$

- The task of turbulence module: Provide μ_T and T_{ij}

- Turbulence Module:

- ◇ Input: U_i, ρ and $\mu \dots$ from the mean flow solver

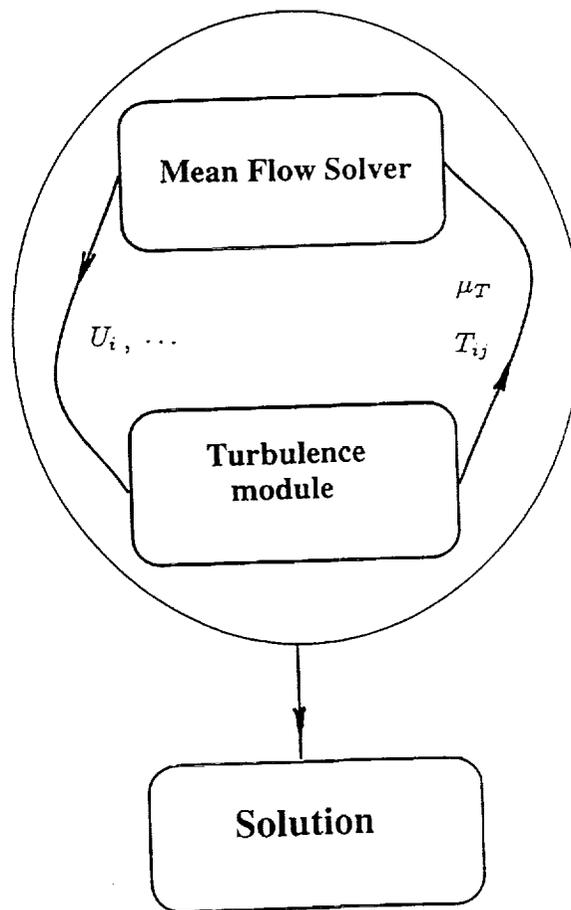
- ◇ Output:

$$\mu_T = C_\mu \frac{k^2}{\varepsilon} \left[\frac{Dk}{Dt} = \dots, \quad \frac{D\varepsilon}{Dt} = \dots \right]$$

$$T_{ij} = -\rho \overline{u_i u_j} - \mu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right)$$

- ◇ Models for $\rho \overline{u_i u_j}$

- One- and two-equation eddy viscosity models
 - Reynolds stress algebraic equation models
 - Reynolds stress transport equation models



Module with CMOTT research code (incompressible)

- CFD equations in CMOTT research code:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} [(\mu + \mu_T) (\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i})] + \frac{\partial}{\partial x_j} T_{ij} - \frac{\partial P}{\partial x_i}$$

- Turbulence module: provide μ_T and T_{ij}
 - ◇ Built-in models without wall function:
 - Launder-Sharma and Chien $k - \epsilon$ models
 - CMOTT $k - \epsilon$ model
 - ◇ Built-in models with wall function:
 - $k - \omega$ model, standard $k - \epsilon$ model
 - CMOTT $k - \epsilon$ model
 - CMOTT Reynolds stress algebraic equation model

Module with NPARC code

- CFD equations in NPARC code:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j} [(\mu + \mu_T) (\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij})] - \frac{\partial P}{\partial x_i}$$

- Turbulence module (present time): provide isotropic μ_T
 - ◇ Build-in models without wall function:
 - Baldwin-Lomax model and Chien $k - \epsilon$ model
 - CMOTT $k - \epsilon$ model
 - ◇ Further development:
 - Models with wall function
 - Reynolds stress algebraic equation models
 - Reynolds stress transport equation models

Joint Program with Industry on Turbulence Module

- For those who want to use the available modules:
 - ◊ Need interface program for particular industry codes
 - Grid informations, Boundary treatment, ...
- For those who want a module for their own codes:
 - ◊ Need modules exclusively for particular industry codes
- Maintain and update the turbulence modules along with model development.

DESCRIPTION OF TURBULENCE SUB-PROGRAM

J. Zhu
Institute for Computational Mechanics in Propulsion
NASA Lewis Research Center
Cleveland, Ohio

General Transport Equations

$$\frac{\partial}{\partial t}(rJ^{-1}\rho\phi) + \frac{\partial}{\partial \xi_i}(C_i\phi - D_i\phi) = rJ^{-1}S_\phi$$

- Non-dimensional form ($\mu, \mu_t \Leftrightarrow \mu/Re, \mu_t/Re$)
- Conservative form
- Cartesian velocity components
 1. Easy to transform (chain rule)
 2. No curvature terms

Discretization

- Finite-volume method

- Source term

$$S_\phi = S_1 + S_2\phi, \quad S_1 \geq 0 \text{ and } S_2 \leq 0$$

- Transient term

1. 1st-order fully implicit scheme
2. 2nd-order three-level fully implicit scheme

- Diffusion term

Standard central differencing scheme

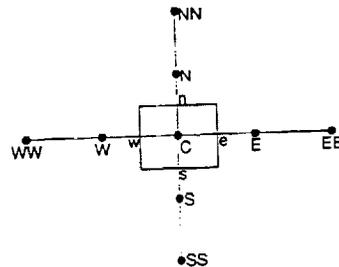
- Convection term: HPLA scheme

(Hybrid Linear/Parabolic Approximation)

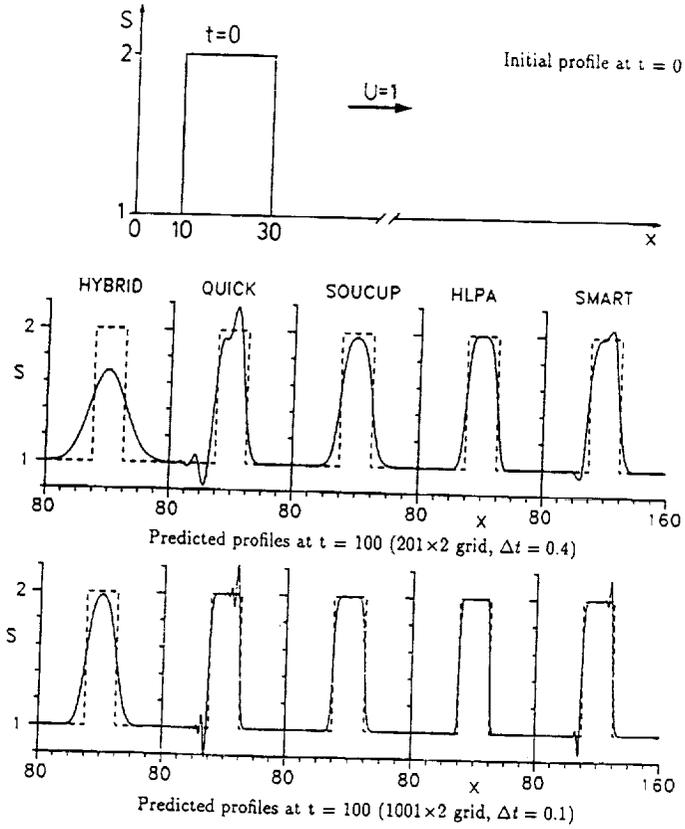
$$\phi_w = \phi_W + \gamma(\phi_C - \phi_W)\hat{\phi}_W, \quad \hat{\phi}_W = \frac{\phi_W - \phi_{WW}}{\phi_C - \phi_{WW}}$$

$$\gamma = \begin{cases} 1 & \text{if } |\hat{\phi}_W - 0.5| < 0.5 \\ 0 & \text{otherwise} \end{cases}$$

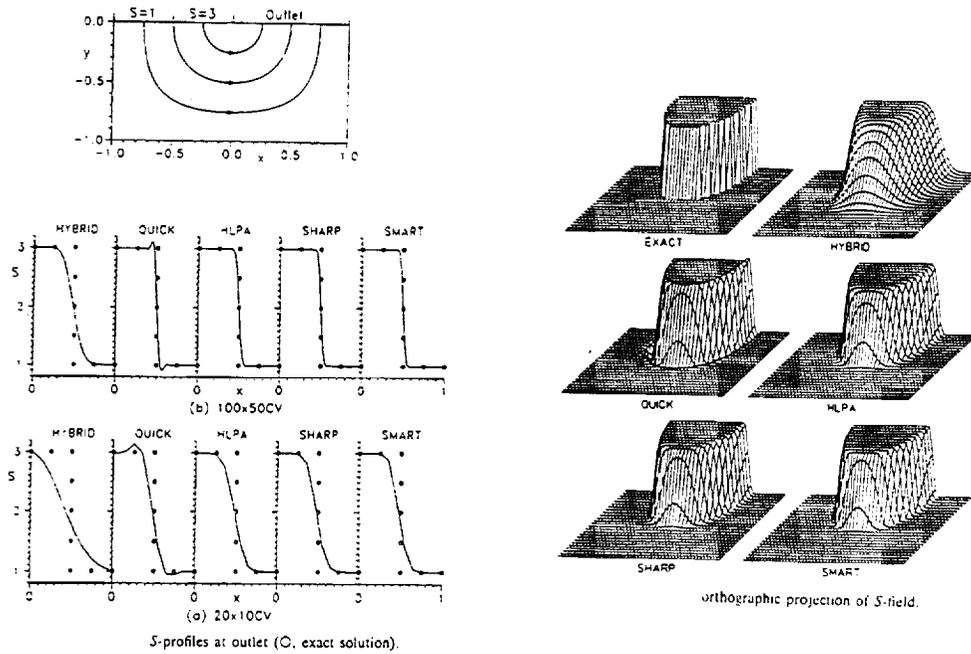
- Second-order accurate
- Bounded (non-oscillatory)
- Diagonally dominant matrix



Example 1



Example 2



Solution Procedure

- Non-delta form
Positiveness ($\phi \geq 0$ but $\Delta\phi$ may < 0)
Simple linearization
- Algebraic equations
$$A_C\phi_C = A_W\phi_W + A_E\phi_E + A_S\phi_S + A_N\phi_N + S$$
$$A's, S \geq 0$$
- Decoupled solution
- Alternating direction TDMA solver

Boundary Conditions

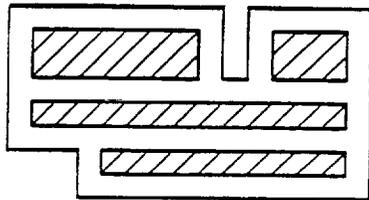
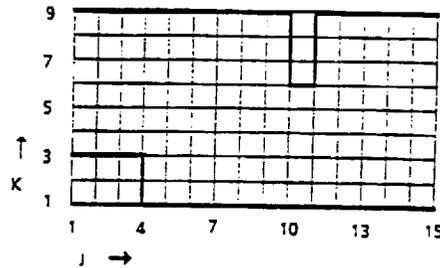
- Inflow: ϕ specified
- Outflow: Fully-developed condition
- Symmetry: $\partial\phi/\partial n = 0$
- Wall:
 1. Low-Reynolds number turbulence models
 2. Standard wall-function approach

Sub-Programs

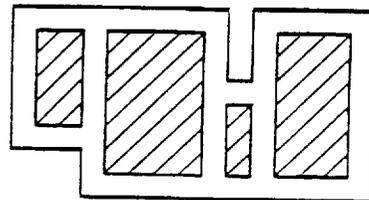
- NPARC2D version
 - Plane or axisymmetric, without swirling
 - Compressible
 - Non-vectorized
- FAST2D version
 - Plane or axisymmetric, with or without swirling
 - Incompressible
 - Vectorized

NPARC2D Version

- Grid arrangement
 - Control volume centers
 - Boundary nodes
 - Embedded bodies



J-Patches



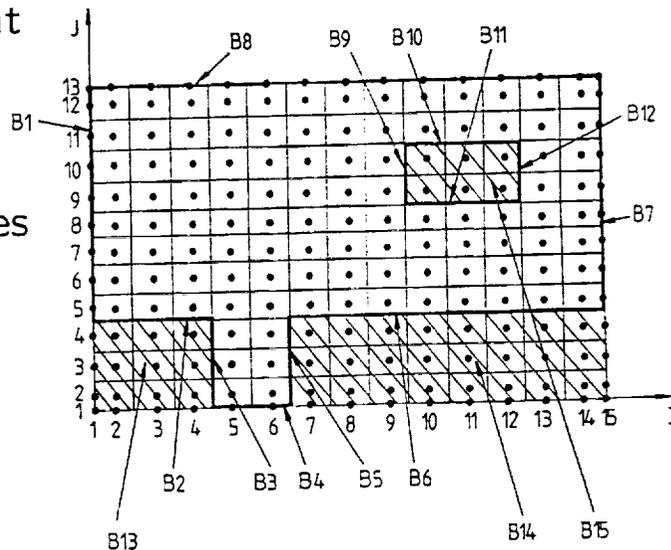
K-Patches

- Input from the main code
 1. Geometric quantities: $x, y, \xi_x, \xi_y, \eta_x, \eta_y, J$
 2. Flow variables: $\mu, J^{-1}\rho, J^{-1}\rho U, J^{-1}\rho V, J^{-1}E$
 3. Patch control: 5×2 parameters
 4. Boundary conditions: 7×2 parameters

- Output
 1. To the main code: μ_t
 2. For post-processing: $K, \epsilon, y^+, y_n, f_\mu$

FAST2D Version

- Grid arrangement
 - CV centers
 - Boundary nodes
 - Embedded bodies



- Vectorization

Single-index:

$$ii = i + (j-1)ni$$

$$\phi(i,j) = \phi(ii)$$

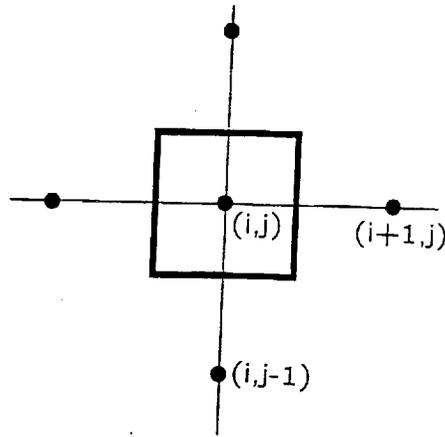
$$\phi(i+1,j) = \phi(ii+1)$$

$$\phi(i,j-1) = \phi(ii-ni)$$

Control parameter:

$$KBLK = \begin{cases} 1 & \text{for computational nodes} \\ 0 & \text{otherwise} \end{cases}$$

$$\phi = KBLK \cdot \phi_c + (1-KBLK) \phi_b$$



- Input from the main code

1. Geometric quantities: $x, y, x_\xi, x_\eta, y_\xi, y_\eta, J$
2. Flow variables: $\mu, \rho, U, V, W, C_w, C_s$
3. Vectorization parameters
4. Boundary parameters

- Output

1. To the main code: μ_t, T_{ij}
2. For post-processing: $K, \epsilon, y^+, y_n, f_\mu$



OVERVIEW OF PROBABILITY DENSITY FUNCTION (PDF) MODELING AT LeRC

D.R. Reddy
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OBJECTIVE

Accurately model the effect of turbulence on
chemical reactions in a fluid flow

APPROACH

Use Probability Density Function (PDF) model -
Express dependent variables as functions
representing statistically realizable events

POSSIBLE MODELING STRATEGIES

1. Evolution PDF - solve for function
 - a. Joint PDF for velocities and chemical species
 - b. Joint PDF for only chemical species
& energy

2. Assumed PDF - function prescribed
Limited range of applicability -
reaction time \ll or \gg turbulence time scale

CURRENT APPROACH

- **Develop evolution PDF model for compressible reacting flows & extend to spray combustion**
- **Solve for joint PDF for species and energy using Monte-Carlo technique**
- **Couple with conventional CFD codes**

AREAS OF IMPACT

- **NO_x Prediction - HSCT and AST application**
- **Spray combustion - swirling turb. reacting flows**
- **Scramjet flow path analysis**
- **Ignition kinetics - prediction of blow-off, etc.**
- **Combustion instability studies**

CODE FEATURES

- **Modular - can be coupled with any CFD code**
- **Applicable for compressible flows with discontinuities**
- **Monte-Carlo solver for generalized curvilinear coordinate system**
- **Easily adaptable for parallel computation (currently under progress)**

CURRENT STATUS

- **2-D and axisymmetric version released (default H₂-air chemistry - 5 species)**
 - parallel version to be released
- **3-D version demonstrated for supersonic combustion (jet in cross flow)**
 - validation planned for HSCT-type configurations
- **General chemistry (CHEMKIN)**
 - Hydrocarbon spray combustion case currently under study
- **CFD codes used - RPLUS, ALLSPD, & SIMPLE-type**

FUTURE PLANS

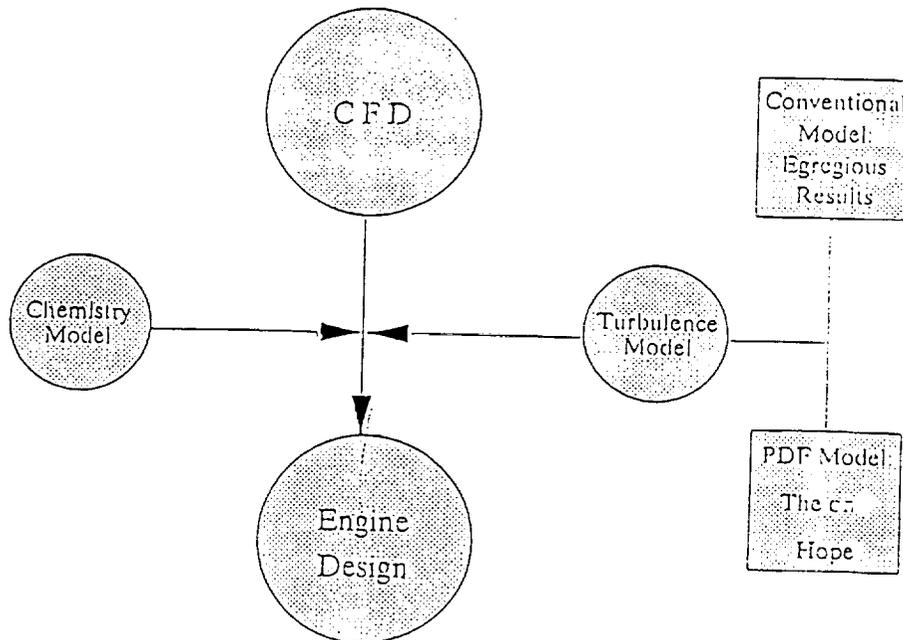
- **Further application/validation of 3-D model**
- **Improved closure models - mixing and turbulence
(use available DNS data)**
- **Parallel processing - workstation clusters**
- **Unsteady applications - long-term**
- **Extend scope of impact**

Andrew T. Hsu
NYMA, Inc.
NASA Lewis Research Center
Brook Park, Ohio

OUTLINE

- . Motivation
- . PDF modeling of reactive flows
- . The Lewis PDF module
- . Validations and applications
- . Current research
- . Technology transfer

COMPUTATION OF TURBULENT COMBUSTION



GOVERNING EQUATIONS

$$\begin{aligned}
 \rho_{,t} + (\rho u_i)_{,i} &= 0 \\
 (\rho u_i)_{,t} + (\rho u_j u_i)_{,j} &= -p_{,i} + \tau_{ij,j} \\
 (\rho E)_{,t} + (\rho u_j E)_{,j} &= -q_{i,i} + \Phi \\
 (\rho Y_k)_{,t} + (\rho u_j Y_k)_{,j} &= (\rho D Y_{k,j})_{,j} + \omega_k
 \end{aligned}$$

$$A_{,t} \equiv \frac{\partial A}{\partial t}$$

$$A_{,j} \equiv \frac{\partial A}{\partial x_j}$$

CLOSURE PROBLEM:

$$\begin{aligned}
 u_i &= \bar{u}_i + u'_i \\
 Y_i &= \bar{Y}_i + Y'_i
 \end{aligned}$$

- $\overline{u'_i u'_j}$ — Turbulence Modeling
- $\overline{Y'_i u'_j}$ — Analogy of shear stress: Diffusion model.
- $\overline{\rho w_i}$ — ???

$$\rho w_i = \rho w(Y_1, \dots, Y_n, T)$$

But in general:

$$\overline{\rho w_i} \neq \rho w(\bar{Y}_1, \dots, \bar{Y}_n, \bar{T})$$

PDF Modeling of Turbulent Reactive Flows Current status

- Assumed PDF (Spalding, 1971; Gosman & Lockwood, 1973; ...)
 - ◊ Advantage: simple, fast.
 - ◊ Disadvantages: Need unique mixture fraction; assumed shape may not be real.
- Composition PDF (Pope, 1976; Dopazo & O'Brian, 1974)
 - ◊ Advantage: Reaction rate treated exactly; existing moment closure codes easily adapted.
 - ◊ Disadvantages: Turbulent diffusion needs model.
- Velocity-Composition joint PDF (Pope & Chen 1980, Pope 1981)
 - ◊ Advantage: Reaction rate treated exactly; no diffusion model needed.
 - ◊ Disadvantages: Models for velocity field relatively untried; Require more computer resource.

PDF Modeling of Turbulent Reactive Flows

- Objective:
 - ◊ Develop models that can accurately simulate finite rate chemical reactions in turbulent flows.
 - ◊ Develop and validate independent PDF modules.
 - ◊ Technology transfer.
- Criteria
 - ◊ Accuracy and robustness.
 - ◊ Practical in terms of today's computing power.
 - ◊ Easy integration with existing industry computational platform.

PDF Modeling of Turbulent Reactive Flows

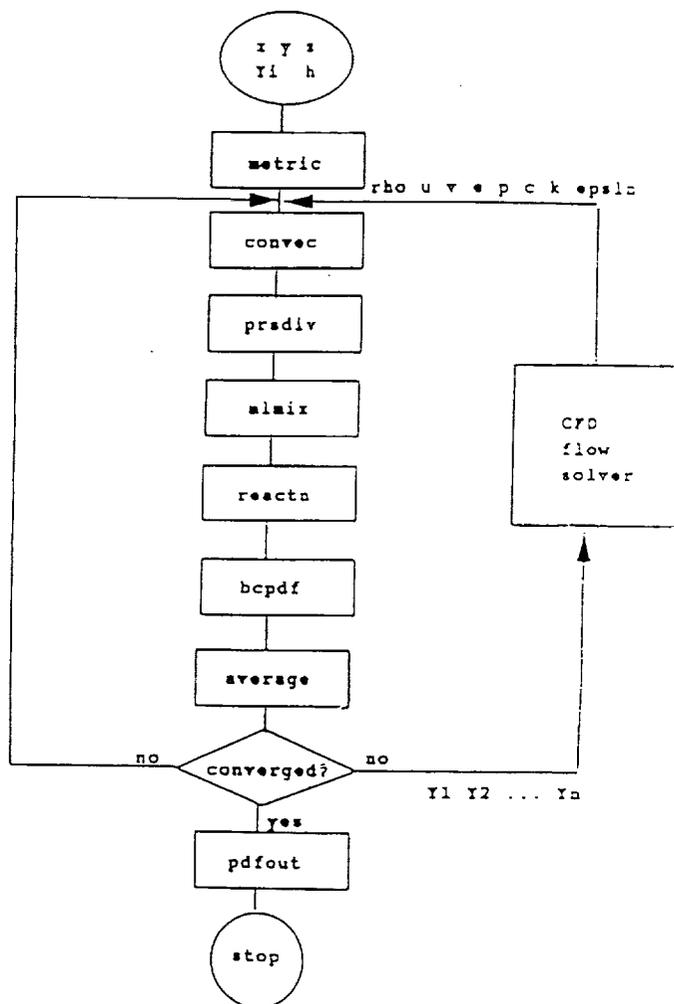
- Approach:
 - ◇ Joint pdf method for scalar compositions.
 - ◇ Moment closure schemes for velocity field.
 - ◇ Develop hybrid solver consisting of Monte Carlo method and finite-difference/finite-volume method.

PDF Modeling of Turbulent Reactive Flows

- Current status (Lewis)

$$\begin{aligned} & (\rho P)_{,t} + (\rho \langle u_j | Y_i, h \rangle P)_{,j} + (\rho w_j P)_{,Y_j} \\ & = (D_t P_{,j})_{,j} + M(P) - (S_\rho P)_{,h}. \end{aligned}$$

- ◇ Continuous mixing model developed.
- ◇ Model for compressibility effect proposed.
- ◇ 2D and 3D Monte Carlo PDF module developed.
- ◇ Validation studies.
- ◇ Code released to industry during a workshop.



Validation Cases

- Scalar field in homogeneous turbulence.
- Oblique shock.
- 2D supersonic hydrogen combustor.
- Axisymmetric supersonic combustor.
- Piloted flame near extinction.

Scalar field in homogenous turbulence pdf compared with Gaussian distribution

Current model

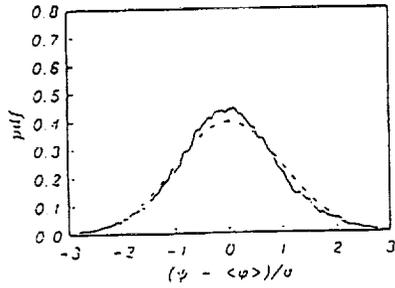


Figure 2. Asymptotic pdf distribution for a scalar in homogeneous turbulence. — present model; - - Gaussian.

Modified curl's model

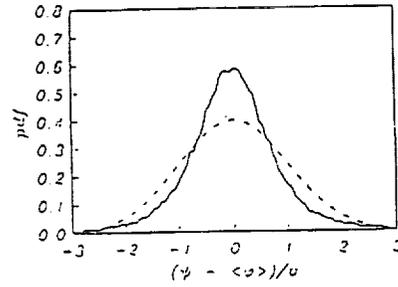
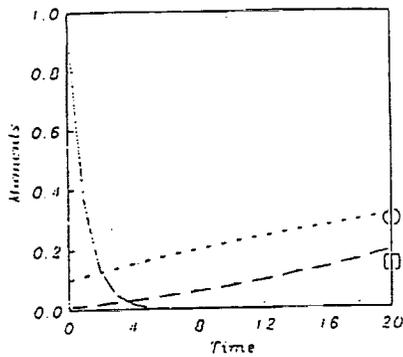


Figure 1. Asymptotic pdf distribution for a scalar in homogeneous turbulence. — modified Curl model; - - Gaussian.

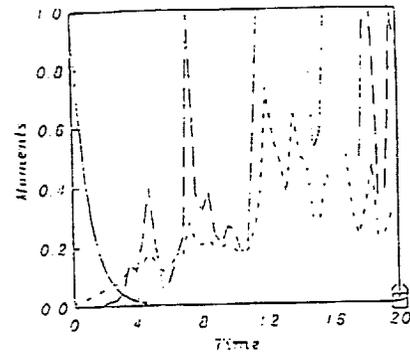
Scalar field in homogenous turbulence 3rd and 4th moments compared with Gaussian

Current model



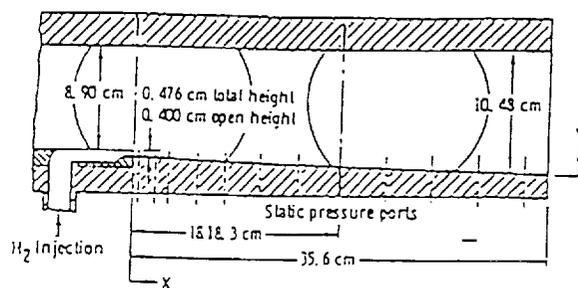
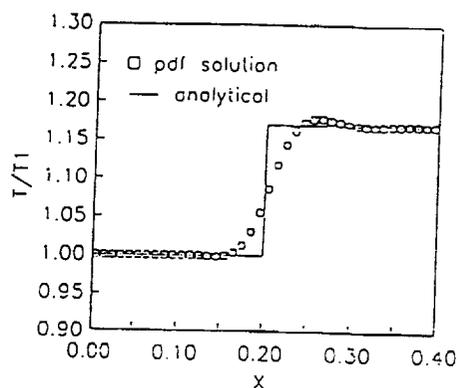
Evolution of moments from the present model. — standard deviation, ···· 0.1 x fourth central moment, - - 0.01 x sixth central moment, ○ 0.1 x fourth moment for Gaussian distribution, □ 0.01 x sixth moment for Gaussian distribution.

Modified curl's model

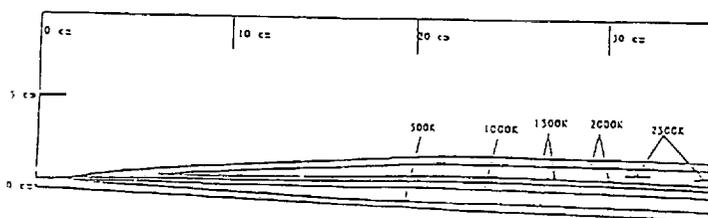


Evolution of moments from the modified Curl model. — standard deviation, ···· 0.01 x fourth central moment, - - 0.0001 x sixth central moment, ○ 0.01 x fourth moment for Gaussian distribution, □ 0.0001 x sixth moment for Gaussian distribution.

Temperature across an oblique shock:
pdf solution compared with analytical
prediction.

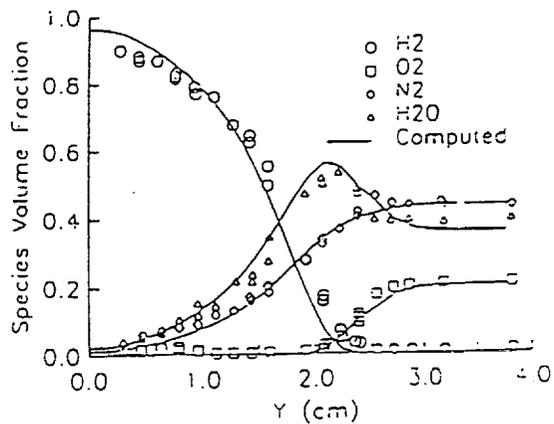


Supersonic hydrogen combustor
(Exp. Burrows & Kurkov, 1973)



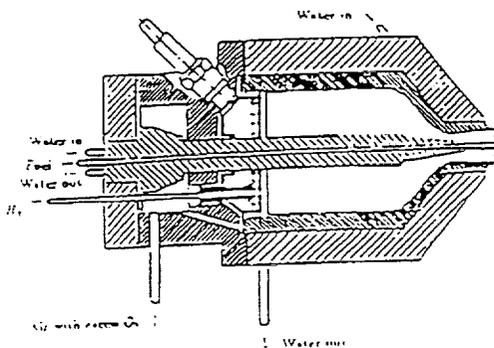
Temperature Contour (pdf solution)

Supersonic hydrogen combustor
 Mole fraction:
 pdf solution compared with exp. data

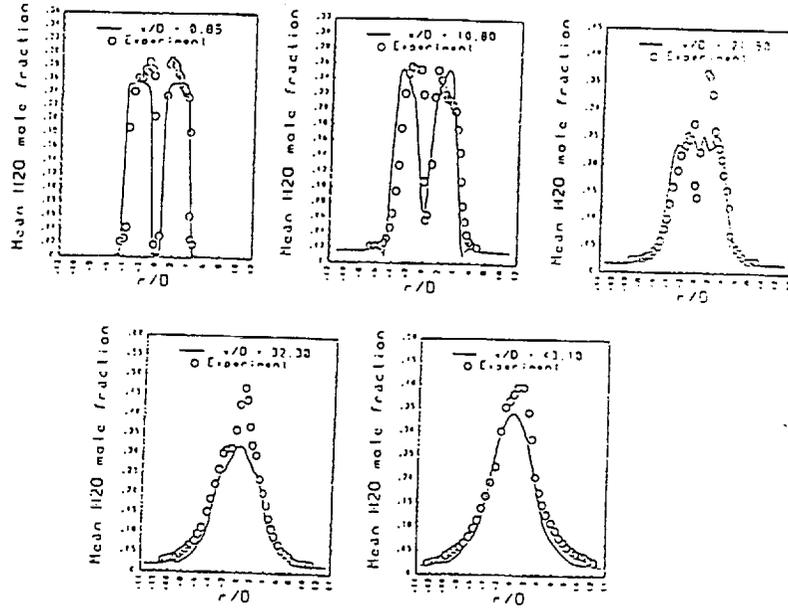


Coaxial burner: geometry and test condition
 (Exp. Cheng, et al. 1991)

Exit Conditions	Hydrogen Jet	Outer Jet	Ambient Air
Mach Number	1	2	0
Temperature, K	545	1250	300
Velocity, m/s	1780	1417	0
Pressure, MPa	.112	.107	.101
Mass Fraction			
Y_{H_2}	1.	0.	0.
Y_{O_2}	0.	.245	.233
Y_{N_2}	0.	.35	.737
Y_{H_2O}	0.	.175	.01

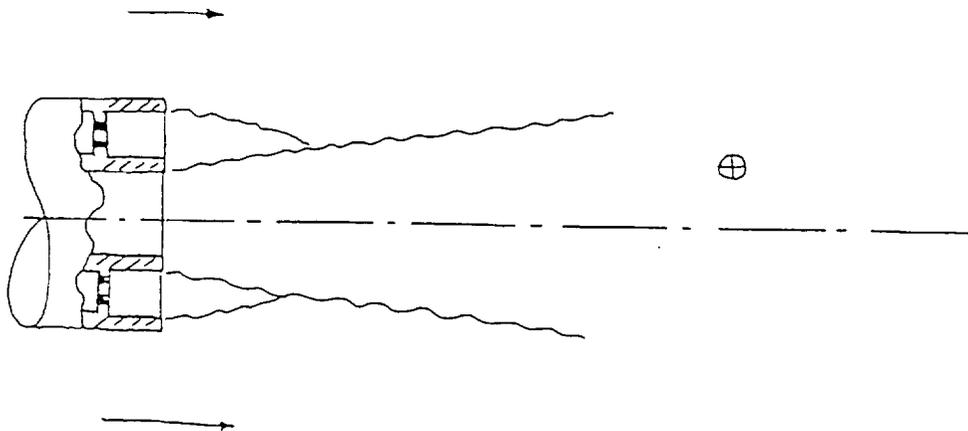


Mean H₂O mole fraction
 Coaxial burner
 pdf solution compared with exp. data

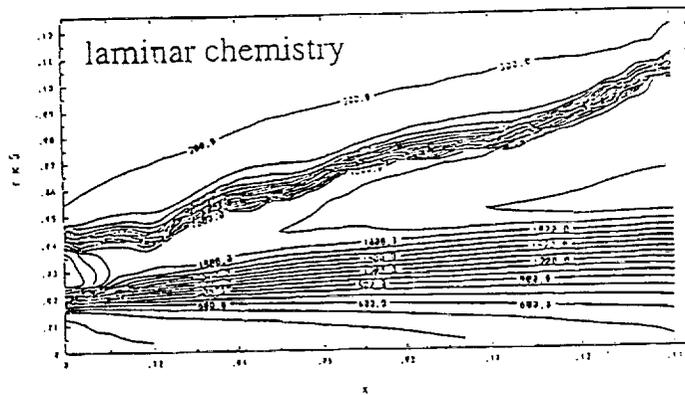
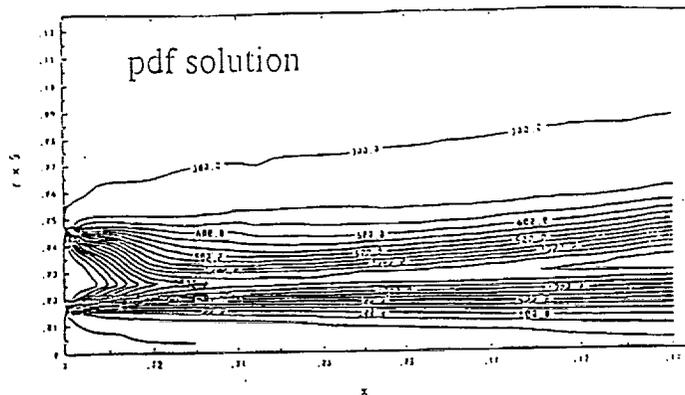


Piloted flame (Masri et al., 1994)

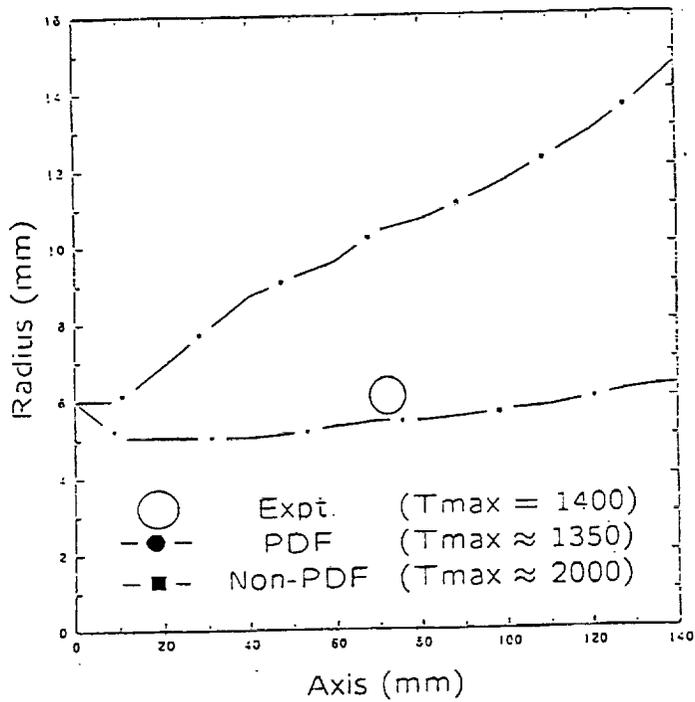
Fuel: 45% CO, 15% H₂, and 40% N₂
 Flame close to extinction



Piloted Flame
Mean Temperature



Piloted Flame
Flame Location



Current Projects

- ◇ Application of PDF module to emission predictions
- ◇ Incorporate general chemistry procedure.
- ◇ Incorporate spray models.
- ◇ Use parallel computing for the PDF module.

Collaboration with industry and technology transfer

- Features of independent pdf module:
 - ◇ Easily coupled with any existing industry flow codes.
 - ◇ Novel averaging scheme to reduce memory requirement.
 - ◇ General chemistry package.
 - ◇ Parallelized workstation version.
- Technology transfer: workshops
 - ◇ July, 1993; code released to 15 US institutions.
 - ◇ October, 1994.



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INTRODUCTION

- THE COMPOSITION JOINT PDF METHOD HAS BEEN USED TO MODEL A WIDE CLASS OF GASEOUS TURBULENT REACTIVE FLOWS. (S.B. POPE)
- NONLINEAR CHEMICAL REACTION RATES COULD BE EVALUATED WITHOUT ANY APPROXIMATION.
- AN EXTENSION OF THE PDF METHOD TO THE MODELING OF SPRAY FLAMES.
- EVALUATE THE LIMITATIONS AND CAPABILITIES OF THIS METHOD IN THE MODELING OF GAS- TURBINE COMBUSTOR FLOWS.

Composition Joint Pdf Transport Equation

$$\begin{aligned} \bar{\rho} \bar{p}_{,t} + \bar{\rho} \bar{u}_i \bar{p}_{,x_i} + [\bar{\rho} w_\alpha(\psi) \bar{p}]_{,\psi_\alpha} = \\ \{ \text{Mean convection} \} \quad \{ \text{Chemical reactions} \} \\ - [\bar{\rho} \langle u_i'' | \underline{\psi} \rangle \bar{p}]_{,x_i} - [\bar{\rho} \langle \frac{1}{\rho} J_{i,x_i}^\alpha | \underline{\psi} \rangle \bar{p}]_{,\psi_\alpha} \\ \{ \text{Turbulent convection} \} \quad \{ \text{Molecular mixing} \} \\ - [\bar{\rho} \langle \frac{1}{\rho} s_\alpha | \underline{\psi} \rangle \bar{p}]_{,\psi_\alpha} \\ \{ \text{Liquid - phase exchange} \} \end{aligned}$$

- \bar{p} = Density-weighted joint pdf.
- w_α = chemical source term for the α -th composition variable.
- $\langle u_i'' | \underline{\psi} \rangle$ = conditional average of Favre velocity fluctuations.
- $\langle \frac{1}{\rho} J_{i,x_i}^\alpha | \underline{\psi} \rangle$ = conditional average of scalar dissipation.
- $\langle \frac{1}{\rho} s_\alpha | \underline{\psi} \rangle$ = conditional average of liquid-phase source term for the α -th composition variable.

Modeling Aspects of the Pdf Transport Equation

- $\langle u_i'' | \underline{\psi} \rangle$ is modeled using a gradient-diffusion model.
- $\langle \frac{1}{\rho} J_{i,x_i}^\alpha | \underline{\psi} \rangle$ is modeled using a variant of Curl's model.
- The new term $\langle \frac{1}{\rho} s_\alpha | \underline{\psi} \rangle$ involving the conditional average of liquid-phase source term is modeled based on the average values of species and enthalpy:

$$\langle \frac{1}{\rho} s_\alpha | \underline{\psi} \rangle = \frac{1}{\bar{\rho} \Delta v} \sum n_k m_k (\epsilon_\alpha - \phi_\alpha)$$

$$\text{for } \phi_\alpha = Y_\alpha, \alpha = 1, 2, \dots, s = \sigma - 1$$

$$\langle \frac{1}{\rho} s_\alpha | \underline{\psi} \rangle = \frac{1}{\bar{\rho} \Delta v} \sum n_k m_k (-l_{k,eff} + h_{k,s} - \phi_\alpha)$$

$$\text{for } \phi_\sigma = h.$$

MODELING ASPECTS

- THE MODELED PDF TRANSPORT EQUATION PROVIDES THE SOLUTION FOR THE SPECIES AND TEMPERATURE FIELDS WITH THE MEAN VELOCITY AND THE TURBULENT DIFFUSIVITY AND FREQUENCY PROVIDED AS INPUTS FROM THE CFD SOLVER AND THE SPRAY SOURCE TERMS FROM THE LIQUID-PHASE SOLVER.
- THE MEAN FLOW AND TURBULENCE EQUATIONS ARE SOLVED BY A CONVENTIONAL CFD SOLVER WITH THE MEAN SPECIES AND TEMPERATURE FIELDS PROVIDED AS INPUTS FROM THE PDF SOLVER AND THE SPRAY SOURCE TERMS FROM THE LIQUID-PHASE SOLVER.
- THE LIQUID-PHASE EQUATIONS ARE FORMULATED IN LAGRANGIAN COORDINATES WITH APPROPRIATE CONSIDERATION TAKEN INTO ACCOUNT OF THE EXCHANGES OF MASS, MOMENTUM, AND ENERGY BETWEEN THE TWO PHASES.

NUMERICAL METHOD

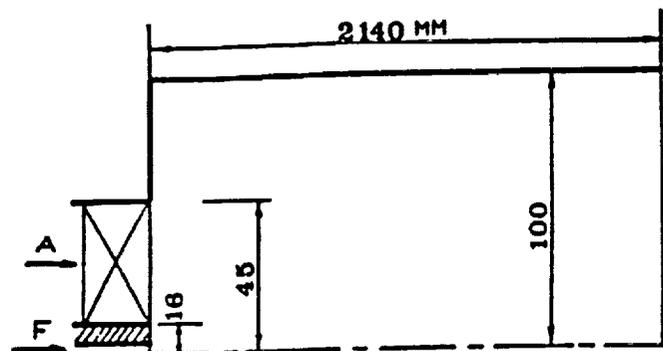
- Mean-Flow and Turbulence Equations
 - Axisymmetric, Unsteady.
 - Incompressible Navier-Stokes (Variable-Density).
 - A Standard Two-Equation k - ϵ Turbulence Model.
 - A Pressure-Based CFD Solver Based on the SIMPLE Algorithm of Patankar and Spalding.
- Liquid-phase Equations
 - The Spray Model (Raju and Sirignano).
 - Dilute Spray Assumption.
 - The ODE's for the Particle Size, Velocity, and Location are Solved Using a R-K Method.
 - The PDE's for the Internal Droplet Distribution (Vortex Model) are Solved by an Implicit Method.
 - Droplet Regression Rate is Based on Either a Gas-Phase Boundary Layer-Analysis or Low-Reynolds Correlation.

NUMERICAL METHOD

- The PDF Transport Equation
 - A Fractional Step Monte-Carlo Method (Pope).
 - Spatial Transport, Molecular Mixing, Liquid-Phase Source Terms, and Chemical Kinetics are advanced in a Series of Sequential Steps.
 - Vectorization
- Interaction Between the Two Phases
 - Interpolation of the Gas-Phase Properties at the Particle Location Using an Area-Weighted Averaging.
 - The Source Terms Evaluated at the Particle Location are redistributed among the surrounding Computational Nodes Using an Area-Weighted Averaging.

CHEMICAL KINETICS MODEL

- IT IS BASED ON A SINGLE STEP GLOBAL MECHANISM OF WESTBROOK AND DRYER FOR N-DECANE/OXYGEN COMBUSTION.
- THIS GLOBAL COMBUSTION MECHANISM WAS SHOWN TO PROVIDE ADEQUATE REPRESENTATION OF TEMPERATURE HISTORIES IN FLOWS NOT DOMINATED BY LONG IGNITION DELAY TIMES.



Geometry of the combustion chamber.
(El Banhawy and Whitelaw)

EXPERIMENTAL DETAILS

- The experimental data corresponds to the following inflow conditions:

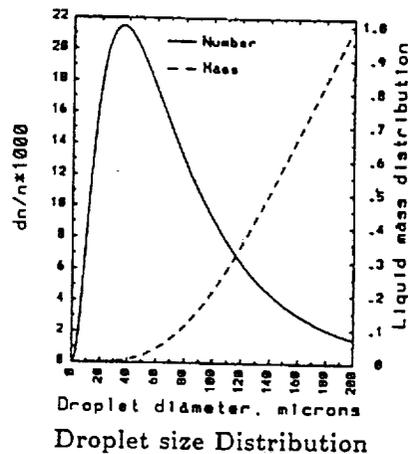
inflow temperature = 310 K,
 air mass flow rate = 355 kg/h,
 air/fuel ratio = 20.17,
 swirl vane angle = 45 deg,
 swirl number = 0.721.

- The reported error in the measurements is about 10 to 15 % for the temperature and about 15% for the velocity.

Details of Fuel Injection

- A fuel nozzle of swirl-atomization type was used.
- The liquid fuel injection is simulated by injecting a discretized parcel of liquid mass at the end of each $\Delta t_{injection}$
- The droplet-size distribution is given by:

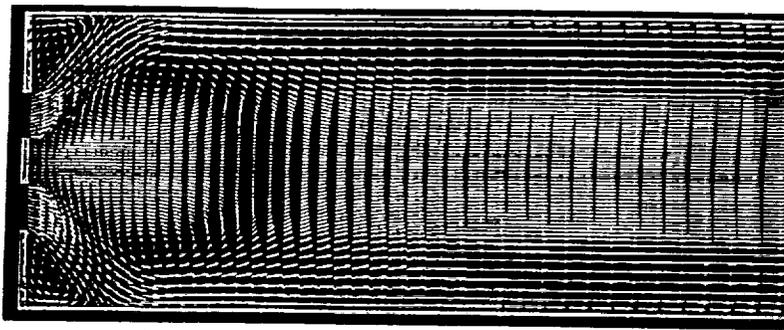
$$\frac{dn}{n} = 4.21 \cdot 10^6 \left[\frac{D}{D_{32}} \right]^{3.5} e^{-16.98 \left(\frac{D}{D_{32}} \right)^{0.4}} \frac{dD}{D_{32}}$$



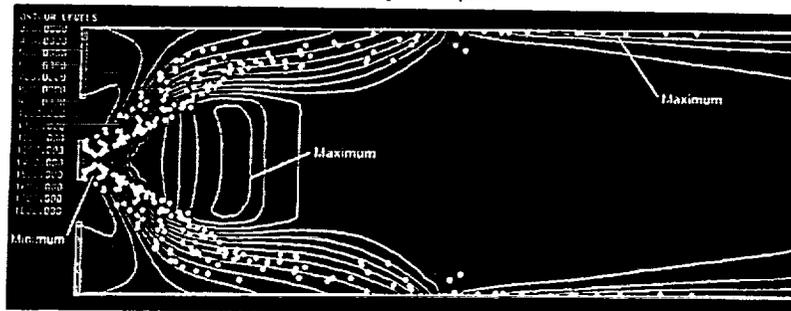
- The initial droplet injection velocity corresponds to: $u_k = 11.0$ m/s, $w_k = 6.1$, and $v_k = 0.5 - 2.5$.

PARAMETER SELECTIONS

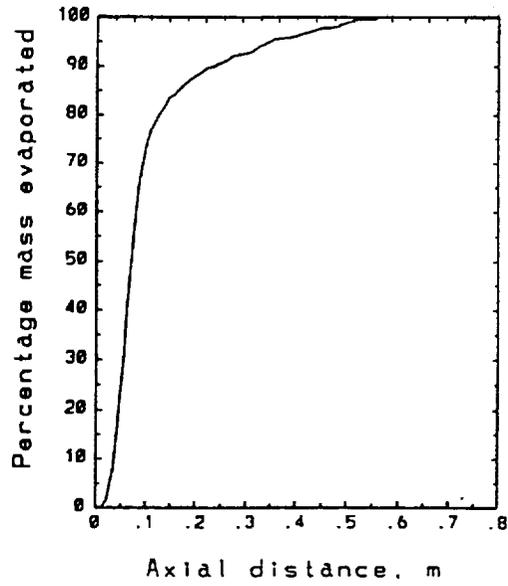
- The computations were performed on a grid with a mesh size of 60x60.
- The PDF solution is obtained by making use of 250 particles per cell.
- $Dt_g = Dt_{\text{injection}} = 1.5 \text{ ms}$, $Dt_k = 0.0375 \text{ ms}$, and $Dt_{\text{Monte-Carlo}} = 0.015 \text{ ms}$.
- Two CPU seconds on a CRAY Y-MP per one Dt_g and about 2 to 3 CPU hours – 4000 time steps – for the solution to reach steady state.



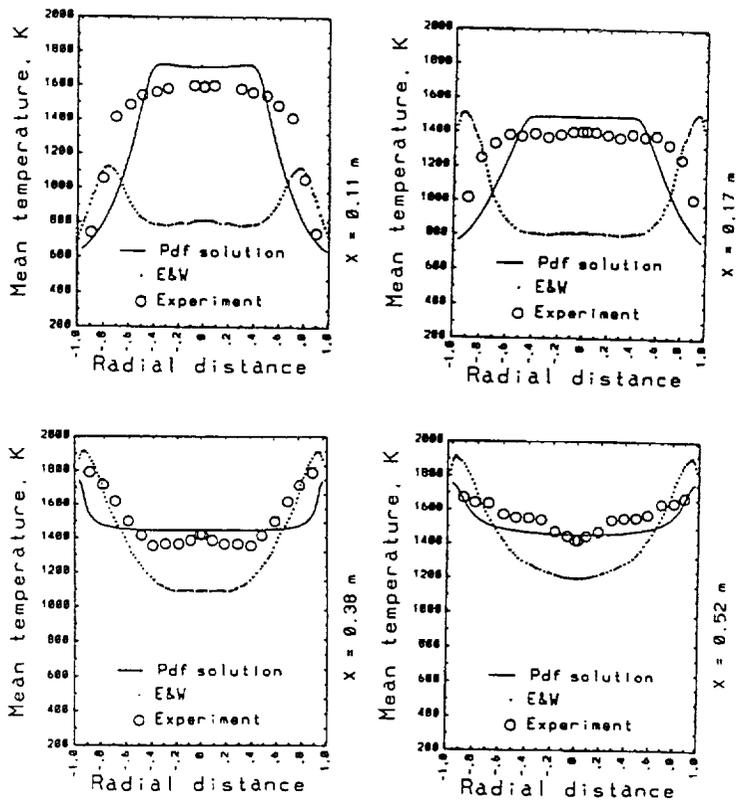
Velocity vector plot.



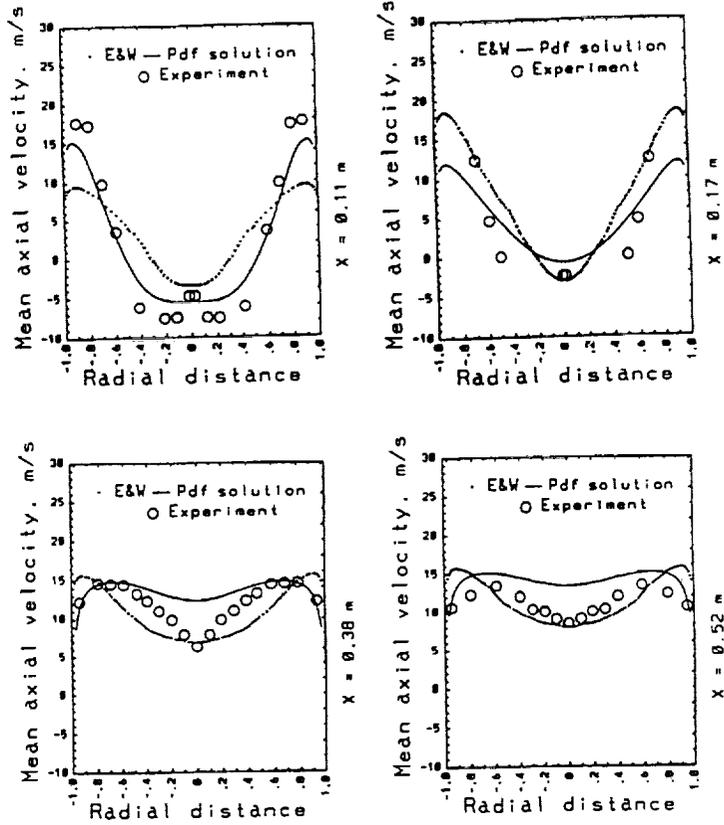
Temperature contours and droplet locations.



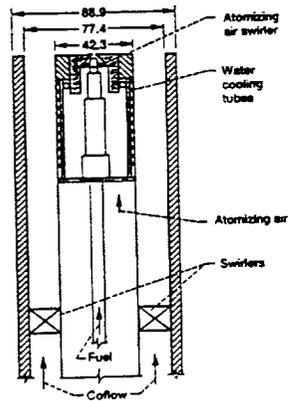
Spray evaporation rate.



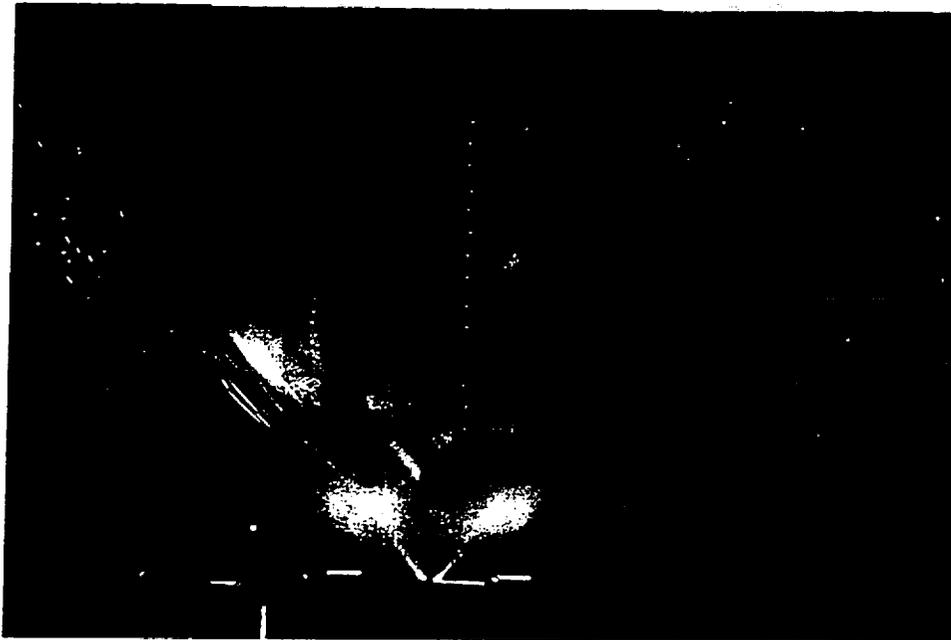
Near wake radial profiles of temperature.



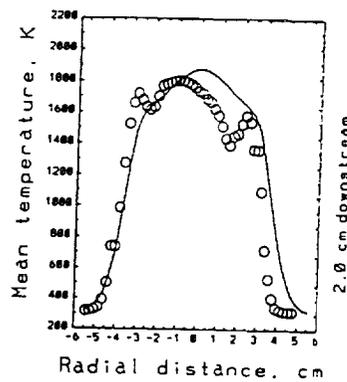
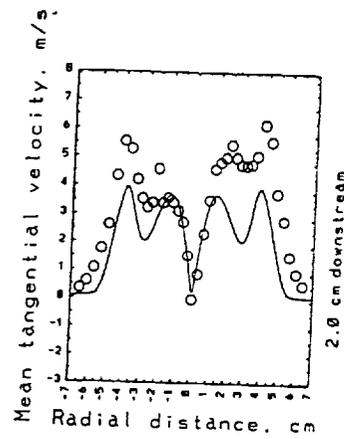
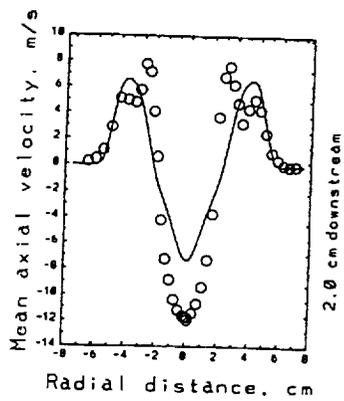
Near wake radial profiles of velocity.

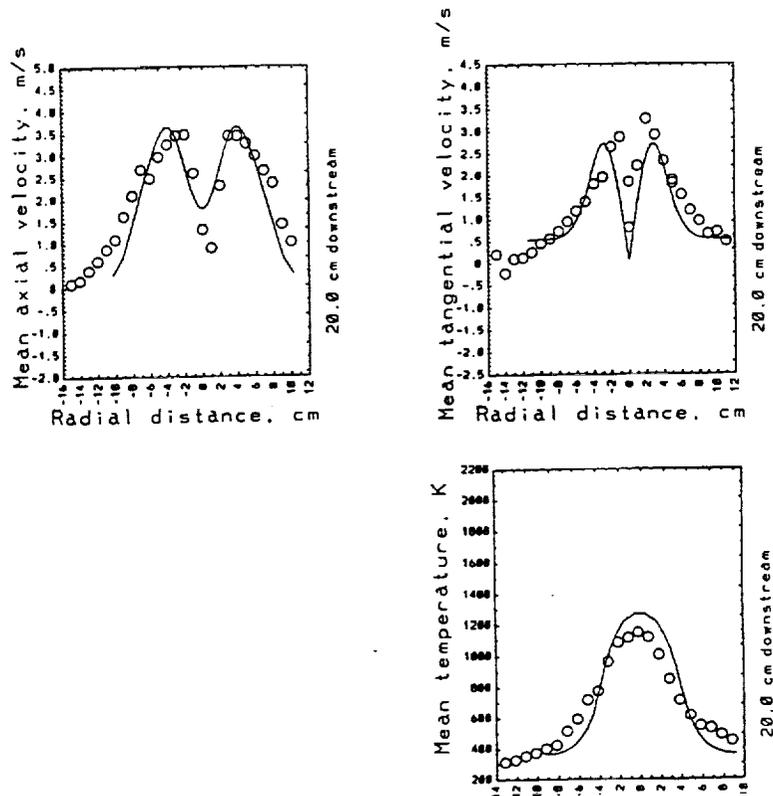


Schematic of an open spray burner.
(Dan Bulzan of IFMD at LeRC)



Photograph of swirl-stabilized, spray flame.





CONCLUDING REMARKS

- The comparisons show that the general features of the flowfield are correctly predicted by the present solution procedure.
- The present solution appears to provide a better representation of the temperature field, particularly, in the reverse-velocity zone.
- The overpredictions in the centerline velocity could be attributed to the following reasons:
 - The use of $k-\epsilon$ turbulence model is known to be less precise in highly swirling flows.
 - The swirl number used here is reported to be estimated rather than measured.

IMPROVEMENTS AND NEW FEATURES IN THE PDF MODULE

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Overview

- Modeling: What models are used in this package and what are their advantages and disadvantages.
- Numerics: Describe how the PDF model is implemented and what are the features of the program.
- Future Developments: What can be expected in the future from the NASA Lewis PDF code.

PDF Modeled Equations.

- Exact scalar PDF transport equation is:

$$\begin{aligned}
 \frac{\partial}{\partial t}(\bar{\rho}P) &+ \frac{\partial}{\partial x_i}(\bar{\rho}\bar{U}_iP) + \frac{\partial}{\partial \phi_\alpha}(\bar{\rho}S_\alpha(\underline{\psi}, p, \eta)P) \\
 &= \frac{\partial}{\partial x_i}(\langle \bar{\rho}\bar{u}_i | \underline{\psi}, \eta \rangle P) + \frac{\partial}{\partial \phi_\alpha}(\langle \frac{\partial J_i^\alpha}{\partial x_i} | \underline{\psi}, \eta \rangle P) \\
 &+ \frac{\partial}{\partial \eta}(\langle \frac{\partial q_i^\alpha}{\partial x_i} | \underline{\psi}, \eta \rangle P) + \frac{\partial}{\partial \eta}(\langle \frac{Dp}{Dt} | \underline{\psi}, \eta \rangle P)
 \end{aligned} \tag{1}$$

- Terms on the LHS exact - need to model the four terms on RHS, corresponding to turbulent convection, molecular mixing and the pressure term.

Turbulent Convection

- This term is modeled as a simple gradient diffusion process.

$$\langle \bar{\rho}\bar{u}_i | \underline{\psi}, \eta \rangle P \approx D_t \frac{\partial P}{\partial \psi_\alpha} \tag{2}$$

- D_t is the turbulent diffusion coefficient, equal to the eddy viscosity. (Assume unity Schmidt)
- Disadvantage: Counter-gradient diffusion known to occur in some pre-mixed flames.

Molecular Mixing.

- Molecular mixing can be viewed as process which changes the shape of the scalar PDF without affecting the mean.
- Molecular mixing is modeled by two models: A coalescence/dispersion model (Hsu and Chen) and a relax-to-mean model (Dopazo).
- Advantages of both models is that they are simple and readily adaptable to any number of scalars.
- Disadvantages are the relative lack of physics in the models.

Pressure Term.

- Pressure term model is based on second order closure models for compressible flows (eg. Sarkar).

$$\begin{aligned} \left\langle \frac{Dp}{Dt} | \psi, \eta \right\rangle \approx & \frac{\partial \langle p \rangle}{\partial t} + \langle U_i \rangle \frac{\partial p}{\partial x_i} + 0.8 \rho \langle k \rangle \frac{\partial \langle U_i \rangle}{\partial x_i} \\ & + 0.15 \rho P_r M_t - 0.2 \rho \epsilon M_t^2 \end{aligned} \quad (3)$$

- Advantages are that model is tried and tested in finite volume codes. Disadvantage is that only the mean pressure can be used for model. Ideally we would like a stochastic process for two state variables.

Numerics

- Solution of scalar PDF transport equation achieved by a particle based Monte Carlo scheme.
- PDF represented by an ensemble of particles, each with a composition and enthalpy.
- PDF evolves by the motion of these particles in physical, scalar and enthalpy space, by exact and modeled processes. eg. Convection, reaction, mixing.
- Statistics (eg. means) obtained by averaging over ensemble of particles.

Numerical Details - Monte Carlo Scheme

- Module based on cell-centered quantities.
- PDF method is a nodal one. ie. All particles reside at the center of the cell, and can move only to neighboring cells.
- Number of particles at each node is the same and the number remains fixed.
- Statistics obtained by averaging over particles at each node, and also by time-averaging.

Numerics - Convection

- Upwind scheme used for mean convection, and central difference for turbulent convection.
- Evolution achieved by moving particles in from adjacent nodes. Particles are selected at random.
- Fractions of particles are treated by random convection.

$$\text{if 6.3 particles then } \begin{cases} 6.0 & 70\% \text{ of the time} \\ 7.0 & 30\% \text{ of the time} \end{cases} \quad (4)$$

Numerics - Reaction

- Although reaction source term treated exactly, several different numerical schemes are needed. Timing figures are for % of time spent in the PDF part of the code on SPARC II workstation.
- No reaction: For scalar mixing calculations.
(Timing: 17.2 %)
- Equilibrium reaction: Assume reaction proceeds at infinite speed. Table of equilibrium composition as a function of mixture fraction obtained from separate CHEMKIN routine.
(Timing: 24.4 %)

Numerics - Reaction Cont.

- One-step global reaction schemes. Westbrook and Dryer global reactions integrated for each time-step.
(Timing: 51.1 %)
- Tabulated reaction increments. Users create their own table of composition increments as a function of scalars using the adaptive tabulation scheme provided, plus the users favourite reduced mechanism.
(Timing: 58.9 %)
- Chemkin full mechanism integration. Very slow and not recommended except for parallel applications.
(Timing: 97.8 %)

Numerics - Averaging

- To reduce statistical error in the evaluation of the mean scalar quantities (without increasing the number of particles per node), time averaging is employed.
- A weighted time average is used to give more weight to recent values and less to those in the far past.

$$\langle\langle\phi\rangle\rangle_t = \frac{1}{w_t + 1}(\langle\phi\rangle_t + w_t\langle\langle\phi\rangle\rangle_{n-1}) \quad (5)$$

$$w_t = c_t(w_{t-1} + 1) \quad (6)$$

Numerics: Misc.

- A portable random number generator is now included in the module, set up for 32 bit machines.
- A time step check is now performed to ensure boundedness of the PDF solution. ie. no negative numbers of particles.
- Rplus/PDF release ported to workstation environment. K-epsilon now standard turbulence model.

Future Work.

- Release of 3D version with new improvements.
- Implimentation of parallel processing for distributed cluster environment. (PVM based)
- Include model for another state variable to close PDF modeling.



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